```
=> fil reg
FILE 'REGISTRY' ENTERED AT 15:42:29 ON 07 DEC 1999
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STRUCTURE FILE UPDATES:   06 DEC  99  HIGHEST RN 250207-49-9
DICTIONARY FILE UPDATES:  06 DEC  99  HIGHEST RN 250207-49-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 13, 1999

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

  POTENTIAL STEREO BOND SEARCH PROBLEM WITH STN EXPRESS WITH DISCOVER!
  5.0 (Windows Only) SEE NEWS 9 FOR DETAILS

=> d que
L2   (    153155)SEA FILE=REGISTRY ABB=ON  16.127.1/RID
L3   (    299075)SEA FILE=REGISTRY ABB=ON  16.138.1/RID
L4   (     14421)SEA FILE=REGISTRY ABB=ON  16.145.1/RID
L5   (    415652)SEA FILE=REGISTRY ABB=ON  16.136.1/RID
L6   (    231917)SEA FILE=REGISTRY ABB=ON  L5 AND N>2 AND NR>1
L7   (    227272)SEA FILE=REGISTRY ABB=ON  ((L2 OR L3 OR L4)) AND NR>1 AND N>1
L8   (    456381)SEA FILE=REGISTRY ABB=ON  L6 OR L7
L9                SCR 1235
L10               SCR 1297
L11               SCR 1332
L12               STR
```
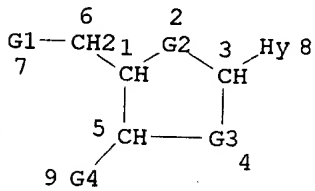
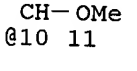
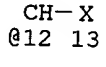
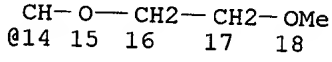
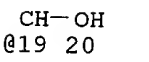









Hy = heterocycle
X = any halogen



full file search done on this structure

```
VAR G1=O/N/S
VAR G2=O/C/N/S
VAR G3=CH2/10/12/14/19
VAR G4=O/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS HIQ  UNS  AT   8
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M2 N  AT   8
```

} heterocycle at 8 is unsaturated & has at least 2 nitrogens

```
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE
L13       112673 SEA FILE=REGISTRY SUB=L8 SSS FUL L12 AND ((L9 OR L10 OR L11))
L14              STR
```

Searched by Barb O'Bryen, STIC 308-4291

subset searches done on the structures that follow

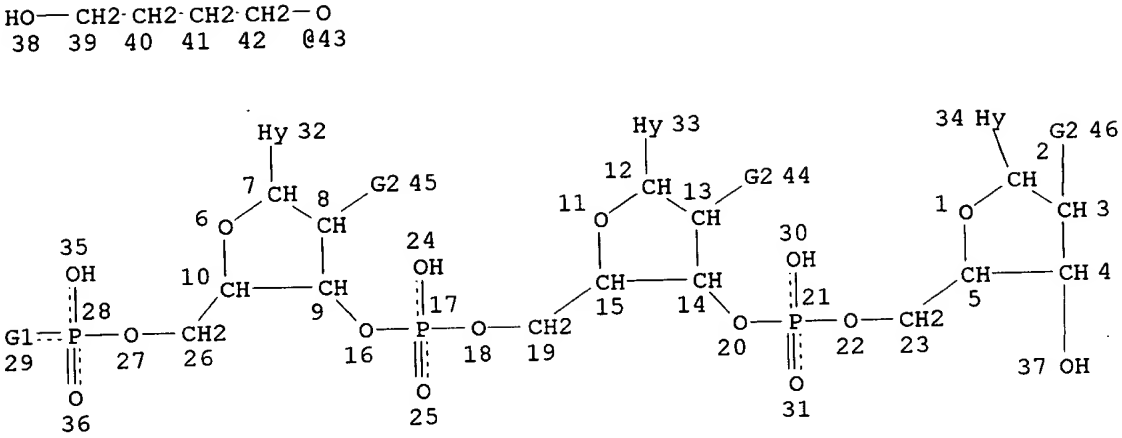
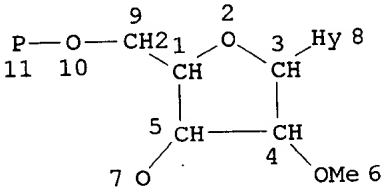


Figure 8

VAR G1=OH/43
VAR G2=OH/OME
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 32
GGCAT IS HIQ UNS AT 33
GGCAT IS HIQ UNS AT 34
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 32
ECOUNT IS M2 N AT 33
ECOUNT IS M2 N AT 34

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 46

STEREO ATTRIBUTES: NONE
L15 STR

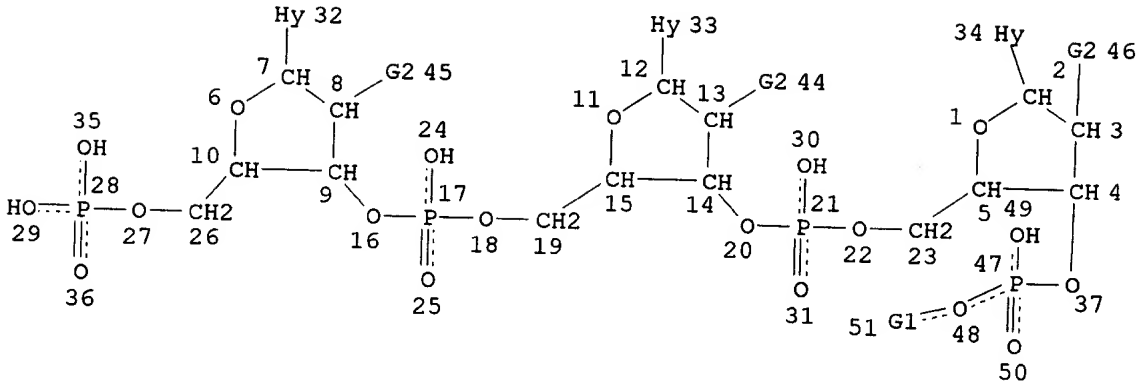


this structure has to be present in answers for Figures 8, 9, 10 (C)

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L16 STR



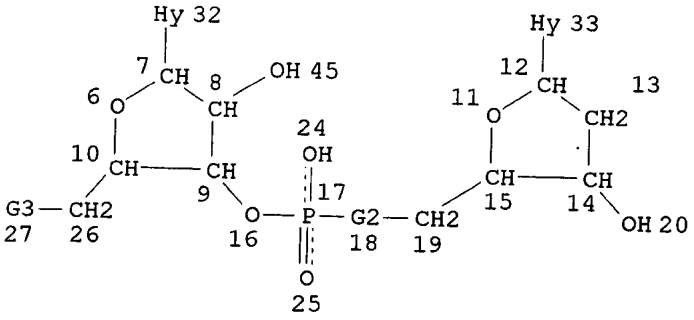
VAR G1=H/N-BU
VAR G2=OH/OME
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 32
GGCAT IS HIQ UNS AT 33
GGCAT IS HIQ UNS AT 34
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 32
ECOUNT IS M2 N AT 33
ECOUNT IS M2 N AT 34

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 45

STEREO ATTRIBUTES: NONE

Figure 9

L17 STR



VAR G2=O/S
VAR G3=SH/OH
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 32
GGCAT IS HIQ UNS AT 33
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 32
ECOUNT IS M2 N AT 33

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

Figure 10 (A)

L18 STR

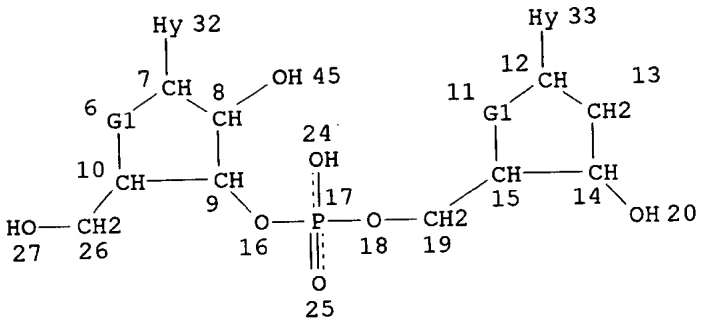
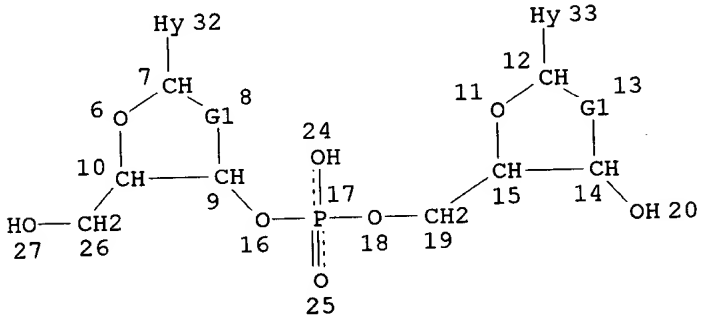


Figure 10 (B)

VAR G1=O/C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 32
GGCAT IS HIQ UNS AT 33
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 32
ECOUNT IS M2 N AT 33

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
L19 STR



CH— OH
@46 47

CH— OMe
@48 49

Figure 10 (C)

VAR G1=CH2/46/48
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 32
GGCAT IS HIQ UNS AT 33
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 32
ECOUNT IS M2 N AT 33

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L20 STR

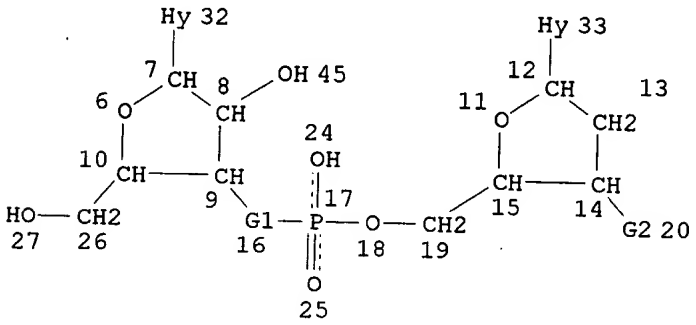


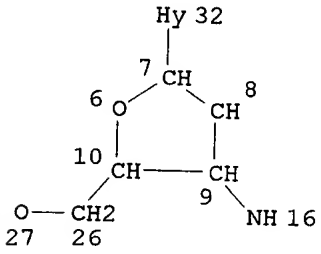
Figure 10 (D)

VAR G1=NH/O
VAR G2=NH/OH
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 32
GGCAT IS HIQ UNS AT 33
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 32
ECOUNT IS M2 N AT 33

(both structures)

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
L21 STR



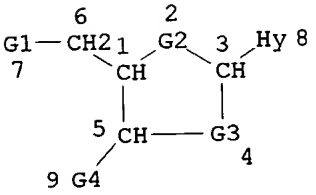
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 32
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 32

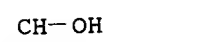
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L23 18 SEA FILE=REGISTRY SUB=L13 SSS FUL ((L14 OR L16 OR L19) AND L15)
L25 32 SEA FILE=REGISTRY SUB=L13 SSS FUL (L17 OR L18)
L26 0 SEA FILE=REGISTRY ABB=ON L25 AND S/ELS Figure 10 (A)
L27 0 SEA FILE=REGISTRY ABB=ON 16.127.1/RID AND L25 Figure 10 (B)
L29 1 SEA FILE=REGISTRY SUB=L13 SSS FUL (L20 AND L21)
L30 (153155) SEA FILE=REGISTRY ABB=ON 16.127.1/RID
L31 (299075) SEA FILE=REGISTRY ABB=ON 16.138.1/RID
L32 (14421) SEA FILE=REGISTRY ABB=ON 16.145.1/RID
L33 (415652) SEA FILE=REGISTRY ABB=ON 16.136.1/RID

Searched by Barb O'Bryen, STIC 308-4291

L34 (231917) SEA FILE=REGISTRY ABB=ON L33 AND N>2 AND NR>1
L35 (227272) SEA FILE=REGISTRY ABB=ON ((L30 OR L31 OR L32)) AND NR>1 AND N>1
L36 (456381) SEA FILE=REGISTRY ABB=ON L34 OR L35
L37 SCR 1235
L38 SCR 1297
L39 SCR 1332
L40 STR



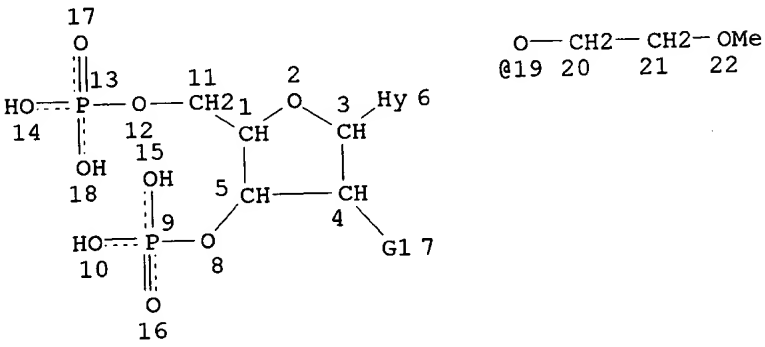


same full file search as on first page

VAR G1=O/N/S
VAR G2=O/C/N/S
VAR G3=CH2/10/12/14/19
VAR G4=O/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS HIQ UNS AT 8
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M2 N AT 8

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L41 (112673) SEA FILE=REGISTRY SUB=L36 SSS FUL L40 AND ((L37 OR L38 OR L39))
L42 STR



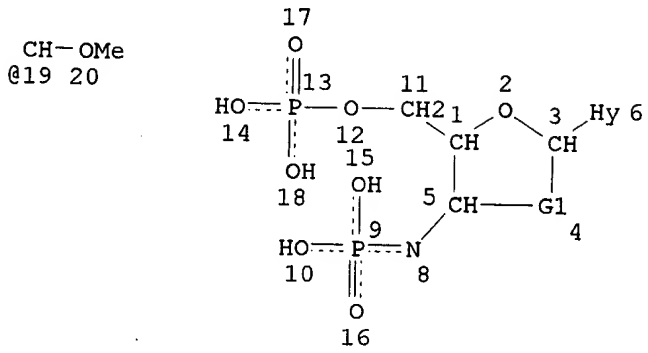
Figures 1, 2, or 3

VAR G1=OME/19/X
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

Searched by Barb O'Bryen, STIC 308-4291

STEREO ATTRIBUTES: NONE
L43 STR

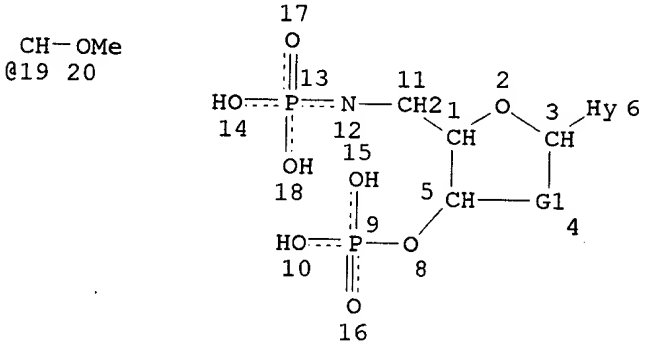


VAR G1=CH2/19
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

Figure 5
(both structures)

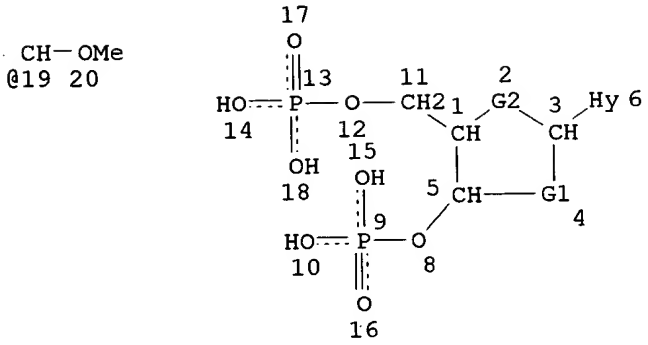
STEREO ATTRIBUTES: NONE
L44 STR



VAR G1=CH2/19
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L45 STR



Figures 6 & 7

VAR G1=CH2/19
VAR G2=S/NH
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L46 STR

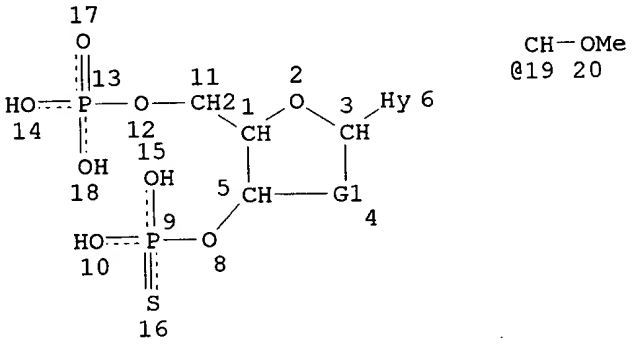


Figure 4

VAR G1=CH2/19
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L47 STR

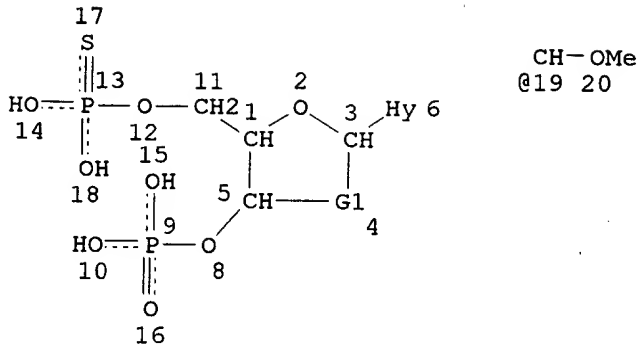


Figure 4

VAR G1=CH2/19
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L48 14 SEA FILE=REGISTRY SUB=L41 SSS FUL (L42 OR L46 OR L47 OR L43 OR L44 OR L45)
L50 33 SEA FILE=REGISTRY ABB=ON L23 OR L26 OR L27 OR L29 OR L48

=> fil capl; s 150
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FILE LAST UPDATED: 6 Dec 1999 (19991206/ED)

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This file supports REGistRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

L51 29 L50

=> d ibib abs hitstr 151 1-29; fil cao; s 150

L51 ANSWER 1 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1999:245290 CAPLUS
DOCUMENT NUMBER: 131:59076
TITLE: Structure-Activity Relationships of Bisphosphate
Searched by Barb O'Bryen, STIC 308-4291

Nucleotide Derivatives as P2Y1 Receptor Antagonists and Partial Agonists

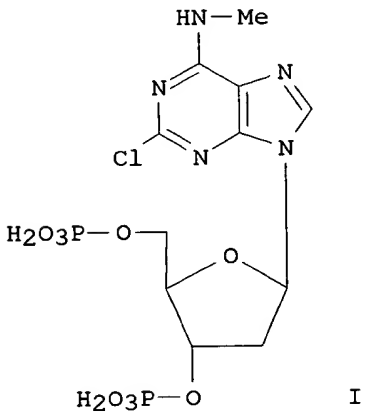
AUTHOR(S): Nandanan, Erathodiyil; Camaioni, Emidio; Jang, Soo-Yeon; Kim, Yong-Chul; Cristalli, Gloria; Herdewijn, Piet; Secrist, John A., III; Tiwari, Kamal N.; Mohanram, Arvind; Harden, T. Kendall; Boyer, Jose L.; Jacobson, Kenneth A.

CORPORATE SOURCE: Molecular Recognition Section Laboratory of Bioorganic Chemistry, National Institute of Diabetes Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0810, USA

SOURCE: J. Med. Chem. (1999), 42(9), 1625-1638
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

AB The P2Y1 receptor is present in the heart, in skeletal and various smooth muscles, and in platelets, where its activation is linked to aggregation. Adenosine 3',5'- and 2',5'-bis-phosphates have been identified as selective antagonists at the P2Y1 receptor and have been modified structurally to increase receptor affinity. We have extended the structure-activity relationships to a new series of deoxyadenosine bis-phosphates with substitutions in the adenine base, ribose moiety, and phosphate groups. The activity of each analog at P2Y1 receptors was detd. by measuring its capacity to stimulate phospholipase C in turkey erythrocyte membranes (agonist effect) and to inhibit phospholipase C stimulation elicited by 10 nM 2-(methylthio)ADP (antagonist effect). 2'-Deoxyadenosine bis-phosphate analogs contg. halo, amino, and thioether groups at the 2-position of the adenine ring were more potent P2Y1 receptor antagonists than analogs contg. various heteroatom substitutions at the 8-position. An N6-methyl-2-chloro analog I, was a full antagonist and displayed an IC50 of 206 nM. On the ribose moiety, 2'-hydroxy, 4'-thio, carbocyclic, and six-membered anhydro-hexitol ring modifications have been prepd. and resulted in enhanced agonist properties. The 1,5-anhydro-hexitol analog was a pure agonist with an EC50 of 3 .mu.M, i.e., similar in potency to ATP 5'-Phosphate groups have been modified in the form of triphosphate, Me phosphate, and cyclic 3',5'-diphosphate derivs. The carbocyclic analog had enhanced agonist efficacy, and the 5'-O-phosphonyl-Me modification was tolerated, suggesting that deviations

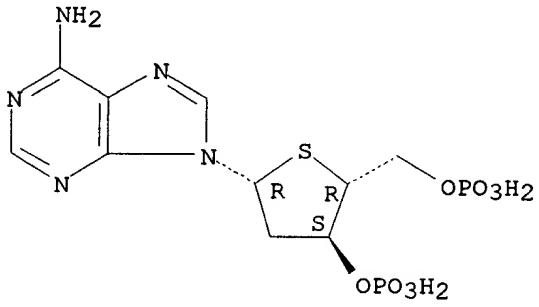
from the nucleotide structure may result in improved utility as pharmacol. probes. The N6-methoxy modification eliminated receptor affinity. Pyrimidine nucleoside 3',5'-bis-phosphate derivs. were inactive as agonists or antagonists at P2Y receptor subtypes.

IT **228264-40-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and structure-activity relationships of bis-phosphate nucleotides as P2Y1 receptor antagonists and partial agonists)

RN 228264-40-2 CAPLUS

CN 3'-Adenylic acid, 2'-deoxy-4'-thio-, 5'-(dihydrogen phosphate), ammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●x NH3

L51 ANSWER 2 OF 29 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1998:618395 CAPLUS

DOCUMENT NUMBER: 129:276239

TITLE: Preparation and normal phase column chromatography purification of DNA

INVENTOR(S): Riley, Timothy Andrew; Reynolds, Mark Alan; Snyder, Lloyd Robert; Klem, Robert E.

PATENT ASSIGNEE(S): Genta, Inc., USA

SOURCE: U.S., 46 pp. Cont.-in-part of U.S. Ser. No. 176,851, abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5811538	A	19980922	US 1994-367069	19941230
PRIORITY APPLN. INFO.:			US 1993-176851	19931230

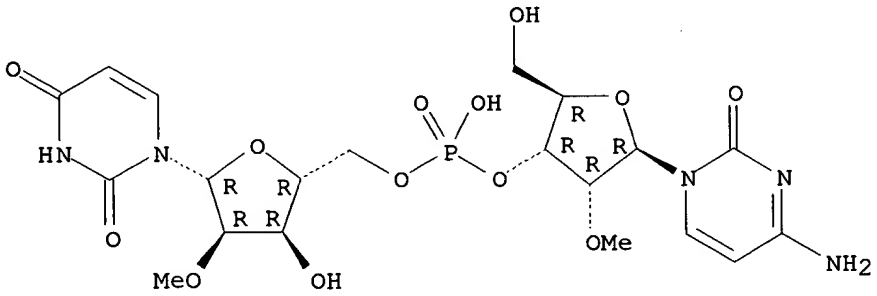
AB Methods for purifying an oligomer by normal phase column chromatog. on a support selected from polyhydroxyethyl aspartamide, hydrophilic silica and silica from an oligomer impurity having a different nucleoside sequence are described. These methods are based upon the different retention times of the oligomer and the impurity on the column.

IT **213690-09-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and normal phase column chromatog. purifn. of DNA)

RN 213690-09-6 CAPLUS

CN Uridine, 2'-O-methylcytidylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

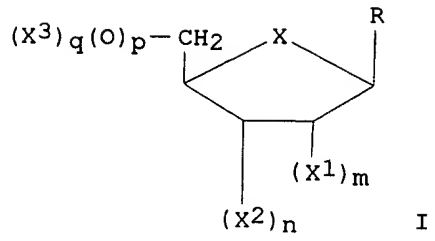
Absolute stereochemistry.



L51 ANSWER 3 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1998:293340 CAPLUS
DOCUMENT NUMBER: 129:4815
TITLE: Preparation and use of nucleotide bis-phosphates as P2Y receptor antagonists
INVENTOR(S): Boyer, Jose L.; Harden, T. Kendall; Jacobson, Kenneth A.; Camaioni, Emidio
PATENT ASSIGNEE(S): University of North Carolina at Chapel Hill, USA; Boyer, Jose L.; Harden, T. Kendall; Jacobson, Kenneth A.; Camaioni, Emidio
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9818430	A2	19980507	WO 1997-US19922	19971023
W: AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, CZ, DE, DE, DK, DK, EE, EE, ES, FI, GB, GE, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2241687	AA	19980507	CA 1997-2241687	19971023
AU 9855846	A1	19980522	AU 1998-55846	19971023
EP 929218	A2	19990721	EP 1997-952172	19971023
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRIORITY APPLN. INFO.:			US 1996-29855	19961030
			WO 1997-US19922	19971023

OTHER SOURCE(S): MARPAT 129:4815
GI



I

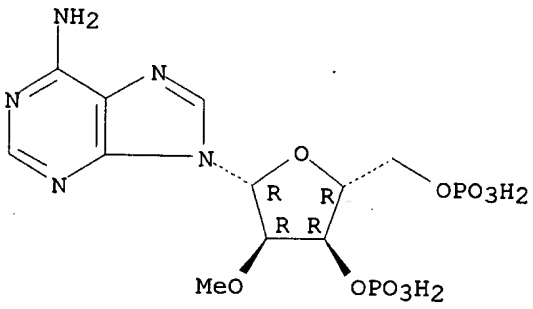
AB Novel P2Y receptor antagonists [(I); R = (un)substituted adenine or uracil, X = O, S, N, CH2; X1, X2, X3 = (independently) H, OH, NH2, alkyl, halo, alkoxy, OPO3H2, OP(S)O2H2, CO2H, NO2, or X1, X2 = -OP(O)(OH)-; m, n = 1-3; p = 0-1; q = 0-3] derived from ATP and UTP are described. P2Y receptor antagonists with competitive antagonist activity at the P2Y receptor are described in particular, as are P2Y receptor antagonists that bind selectively to the P2Y1 receptor. Also described herein are methods of detecting a P2Y receptor in a biol. sample. Thus, 2'-deoxyadenosine was reacted with phosphorous oxychloride to give I (R = adenine; X = O; X1 = H; X2 = OPO3H2; X3 = PO3H2; m, n, p, q = 1)(II) as the tetra-ammonium salt. In in vitro agonist/antagonist expts. using turkey erythrocyte P2Y1 receptors, II had agonist effect of 12.+-.3% at EC50 6.26.+-.2.52 .mu.M, and antagonist effect (measured against 2-methylthio-ATP) of 87.+-.4% at IC50 5.76.+-.0.68 .mu.M.

IT **201048-92-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and use of nucleotide bis-phosphates as P2Y receptor antagonists)

RN 201048-92-2 CAPLUS

CN 3'-Adenylic acid, 2'-O-methyl-, 5'-(dihydrogen phosphate), tetraammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●4 NH_3

L51 ANSWER 4 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1998:9221 CAPLUS
DOCUMENT NUMBER: 128:84049
TITLE: Deoxyadenosine Bisphosphate Derivatives as Potent Antagonists at P2Y1 Receptors
Searched by Barb O'Bryen, STIC 308-4291

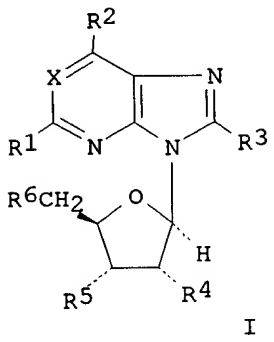
AUTHOR(S): Camaioni, Emidio; Boyer, Jose L.; Mohanram, Arvind; Harden, T. Kendall; Jacobson, Kenneth A.

CORPORATE SOURCE: Molecular Recognition Section Laboratory of Bioorganic Chemistry National Institute of Diabetes Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0810, USA

SOURCE: J. Med. Chem. (1998), 41(2), 183-190
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

AB Adenosine 3',5'- and 2',5'-bisphosphates previously were demonstrated to act as competitive antagonists at the P2Y1 receptor (Boyer et al., 1996). 2'- And 3'-Deoxyadenosine bisphosphate analogs, e.g. I (R1 = R3 = R4 = H, R2 = NH2, R5 = R6 = PO4H2, X = N, N+Me; R1 = Cl, SMe, R2 = NH2, R3 = R4 = H, R5 = R6 = PO4H2, X = N; R1 = R4 = H, R2 = NH2, R3 = Br, R5 = R6 = PO4H2, X = N; R1 = R3 = R4 = H, R2 = NHMe, NHEt, NHPr, NHCOPh, NMe2, Cl, OH, SMe, R5 = R6 = PO4H2, X = N; R1 = R3 = R5 = H, R2 = NH2, NHMe, R4 = R6 = PO4H2, X = N; R1 = R3 = R4 = H, R2 = NH2, R5 = PO4H2, R6 = Cl, X = N; R1 = R3 = H, R2 = NH2, R4 = OMe, R5 = R6 = PO4H2, X = N; R1 = R3 = R4 = H, R2 = NH2, R5 = R6 = PSO3H2, X = N), contg. various structural modifications at the 2- and 6-positions of the adenine ring, on the ribose moiety, and on the phosphate groups have been synthesized with the goal of developing more potent and selective P2Y1 antagonists. Single-step phosphorylation reactions of adenosine nucleoside precursors were carried out. The activity of each analog at P2Y1 receptors was detd. by measuring its capacity to stimulate phospholipase C in turkey erythrocyte membranes (agonist effect) and to inhibit phospholipase C stimulation elicited by 10 nM 2-MeSATP (antagonist effect). Both 2'- and 3'-deoxy modifications were well tolerated. The N6-Me modification both enhanced antagonistic potency (IC50 330 nM) of 2'-deoxyadenosine 3',5'-bisphosphate by 17-fold and eliminated residual agonist properties obsd. with the lead compds. The N6-Et modification provided intermediate potency as an antagonist, while the N6-Pr group completely abolished both agonist and antagonist properties. 2-Methylthio and 2-chloro analogs were partial agonists of intermediate potency. A 2'-methoxy group provided intermediate potency as an antagonist while enhancing agonist activity. An N1-Me analog was a weak antagonist with no agonist activity. An 8-bromo substitution and replacement of the N6-amino group with methylthio, chloro, or hydroxy groups greatly reduced the ability to interact with P2Y1 receptors. Benzoylation or dimethylation of the N6-amino group also abolished the antagonist activity. In summary, our results further define the structure-activity of adenosine bisphosphates as P2Y1 receptor antagonists and have led to the identification of the most potent antagonist reported

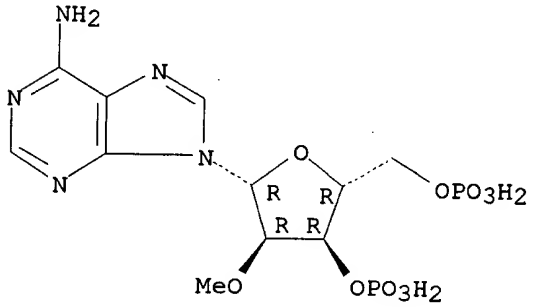
to date for this receptor.

IT **201048-92-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of deoxyadenosine bisphosphate derivs. as potent antagonists at P2Y1 receptors)

RN 201048-92-2 CAPLUS

CN 3'-Adenylic acid, 2'-O-methyl-, 5'-(dihydrogen phosphate), tetraammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●4 NH_3

L51 ANSWER 5 OF 29 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1997:743633 CAPLUS

DOCUMENT NUMBER: 128:34969

TITLE: Synthesis of 3'-thioribonucleosides and their incorporation into oligoribonucleotides via phosphoramidite chemistry

AUTHOR(S): Sun, Sengen; Yoshida, Aiichiro; Piccirilli, Joseph A.

CORPORATE SOURCE: Howard Hughes Medical Institute, Department of Biochemistry and Molecular Biology, The University of Chicago, Chicago, IL, 60637, USA

SOURCE: RNA (1997), 3(11), 1352-1363
CODEN: RNARFU; ISSN: 1355-8382

PUBLISHER: Cambridge University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

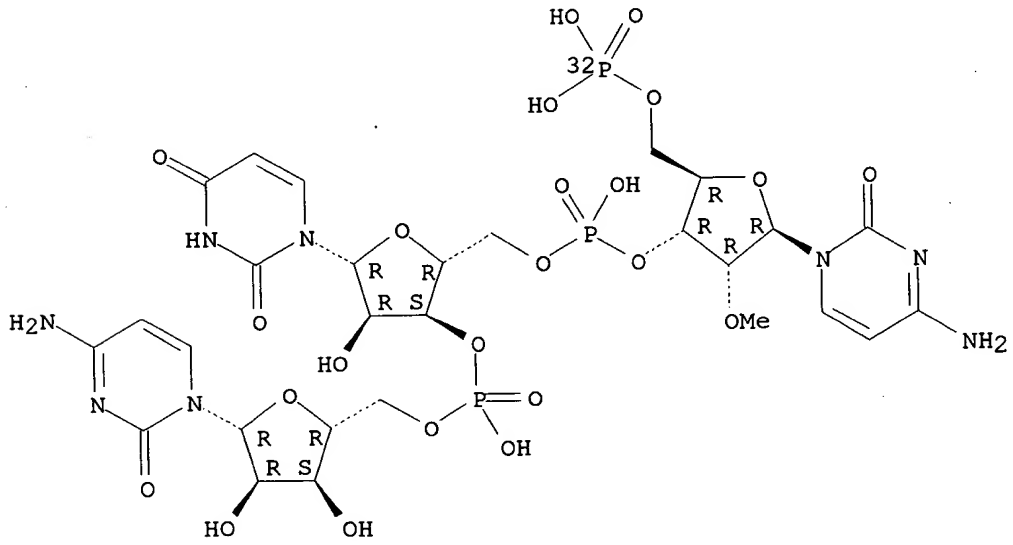
AB Oligoribonucleotides contg. 3'-S-phosphorothiolate linkages are valuable probes in nucleic acid biochem., but their accessibility has been limited because 3'-thioribonucleoside phosphoramidites have not been available. We synthesized 3'-thioribonucleoside derivs. (C, G, and U) via glycosidations of nucleoside bases with 3-S-thiobenzoyl-5-O-toluoyl-1,2-O-diacetylfuranose, which was obtained from 1,2-O-isopropylidene-5-O-toluoyl-3-trifluoromethane-sulfonyl-.alpha.-D-xylofuranose by SN2 displacement with sodium thiobenzoate. Addnl., a 3'-thioinosine deriv. was prepd. from inosine via direct modification of the ribose, analogous to the previously reported synthesis of 3'-thioadenosine, except that the intermediate 2',3'-epoxide 9 was first protected as the 5'-O-tert-butyldiphenylsilyl ether prior to subsequent synthetic steps. This hydrophobic silyl group facilitated extn. and isolation of synthetic intermediates. After removal of the protecting groups, the 3'-thionucleosides (C, G, U, and I) were treated with 2,2'-dipyridyl disulfide to protect the free thiol group as a disulfide. The 3'-thionucleosides were converted to the corresponding phosphorothioamidites using procedures analogous to those for std.

phosphoramidites. The amino groups of 3'-thiocytidine and 3'-thioguanosine were protected as benzoyl and isobutyryl amides, resp., and the 5'- and 2'-hydroxyl groups of each nucleoside were protected as dimethoxytrityl and tert-butyldimethylsilyl ethers, resp. The 3'-thiol group was deprotected by redn. with DTT and phosphitylated to afford anal. pure 3'-S-phosphorothioamidites 15, which were incorporated into oligoribonucleotides by solid-phase synthesis. Chem. assays and mass spectrometry of the synthetic RNA showed that ribose-3'-S-phosphorothiolate linkages were installed correctly and efficiently into RNA oligonucleotides using phosphoramidite chem.

IT **199600-11-8P**
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of thioribonucleosides and their incorporation into oligoribonucleotides via phosphoramidite chem.)

RN 199600-11-8 CAPLUS
CN Cytidine, 2'-O-methyl-5'-O-(phosphono-32P)cytidylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 6 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1996:54407 CAPLUS
DOCUMENT NUMBER: 124:139500
TITLE: Inhibition of HIV-1 RNase H activity by nucleotide dimers and monomers
AUTHOR(S): Allen, S. J. W.; Krawczyk, S. H.; McGee, L. R.; Bischofberger, N.; Mulato, A. S.; Cherrington, J. M.
CORPORATE SOURCE: Gilead Sciences, Inc., Foster City, CA, 94404, USA
SOURCE: Antiviral Chem. Chemother. (1996), 7(1), 37-45
CODEN: ACCHEH; ISSN: 0956-3202
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Nucleotide dimers and monomers were shown to inhibit human immunodeficiency virus type 1 (HIV) RNase H activity. Several effective inhibitors were identified and placed into three general groups based on biochem. characterization of their inhibition. The first group (group A) inhibited HIV RNase H and the closely related feline immunodeficiency virus (FIV) RNase H, but did not inhibit less related retroviral or cellular RNases H or HIV reverse transcriptase (RT). The second group

(group B) inhibited the RNase H activity of several retroviruses as well as the reverse transcriptase function of HIV RT. The third group (group C) inhibited RNases H from retroviral and cellular sources but did not inhibit HIV RT. Kinetic analyses of HIV RNase H inhibition were conducted and all three types of inhibitors exhibited a competitive mode of inhibition with regard to substrate. The small nucleotides described here represent the most potent (Ki values from 0.57 to 16 .mu.M) and selective inhibitors of HIV RNase H reported to date. Further structure - function analyses of these mols. may lead to the discovery of unique, potent antiretroviral therapeutics.

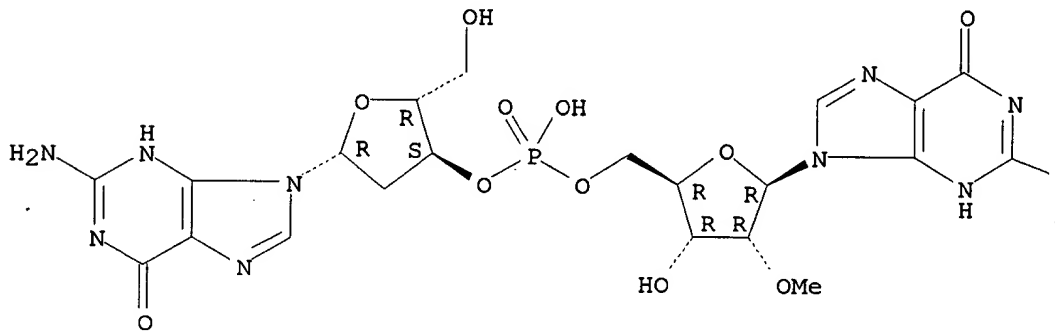
IT **173291-37-7**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(inhibition of HIV-1 RNase H activity by nucleotide dimers and monomers)

RN 173291-37-7 CAPLUS

CN Guanosine, 2'-deoxyguanylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

NH2

L51 ANSWER 7 OF 29 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1995:687098 CAPLUS

DOCUMENT NUMBER: 124:9334

TITLE: Method for the treatment of protozoa infections with 2'-deoxy-2'-fluoropurine nucleosides

INVENTOR(S): Tisdale, Sylvia M.; Van, Tuttle Joel; Slater, Martin J.; Daluge, Susan M.; Miller, Wayne H.; Krenitsky, Thomas A.; Koszalka, George W.

PATENT ASSIGNEE(S): Burroughs Wellcome Co., USA

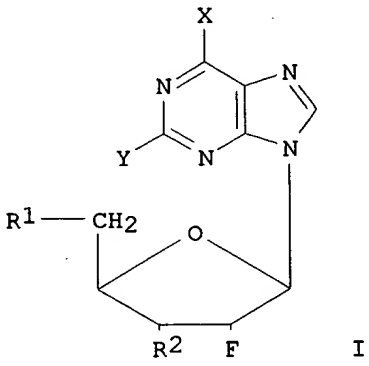
SOURCE: U.S., 21 pp. Cont. of u.S. Ser. No. 580, 105, abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent
Searched by Barb O'Bryen, STIC 308-4291

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5420115	A	19950530	US 1992-940304	19920902
			US 1990-580105	19900910

PRIORITY APPLN. INFO.:
OTHER SOURCE(S): MARPAT 124:9334
GI



I

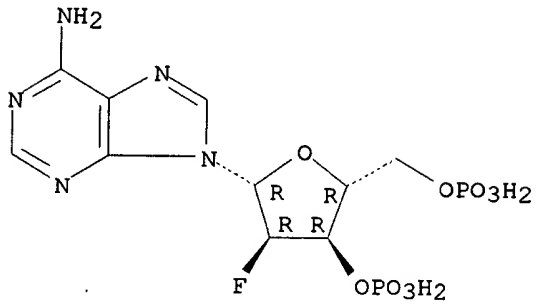
AB 2'-Deoxy-2'-fluoropurine nucleosides I wherein: Y = N, NH2; X is a group NR3R4 in which R3 and R4 may be the same or different and each represent hydrogen, C1-6 alkyl, C2-6 alkenyl, C3-7 cycloalkyl, each group optionally being substituted by one or more halogen, or X is a group ZR5 in which Z is oxygen or sulfur and R5 has the same definition as R3, or X is halogen or hydrogen; R1 and R2, which may be the same or different, each represent: e.g., a hydroxy group; a group OCOR6H where R6 is a divalent group which is straight or branched C1-6 alkylene, C2-6 alkenylene or C3-7 cycloalkylene, each being optionally substituted by one or more hydroxy groups; and their pharmaceutically acceptable salts are anti-infective agents, particularly against viruses [influenza virus, particularly influenza A and B and RSV (respiratory syncytial virus) infections], and certain protozoa, for example, Trichomonas vaginalis and Giardia lamblia. Trichomonas vaginalis and Giardia lamblia are infections are treated by administration to a mammal in need thereof one of the following purine nucleosides: 2,6-diamino-9-(2-deoxy-2-fluoro-.beta.-D-ribofuranosyl)-9H-purine, 2-amino-9-(2-deoxy-2-fluoro-.beta.-D-ribofuranosyl)-9H-purine, and 2-amino-9-(2-deoxy-2-fluoro-.beta.-D-ribofuranosyl)-6-methoxy-9H-purine. Reaction of 1-(2-deoxy-2-fluoro-.beta.-D-ribofuranosyl)uracil with 2,6-diaminopurine in potassium phosphate buffer which contained potassium azide, thymidine phosphorylase, and purine nucleoside phosphorylase afforded 2,6-diamino-9-(2-deoxy-2-fluoro-.beta.-D-ribofuranosyl)-9H-purine which exhibited anti-influenza activity of IC50 = 0.6 .mu.M. Pharmaceutical formulations were given.

IT **134444-67-0P**, 9-(2-Deoxy-2-fluoro-.beta.-D-ribofuranosyl)adenine-3',5'-bisphosphate
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(treatment of protozoa, influenza, and respiratory syncytial virus infections with 2'-deoxy-2'-fluoropurine nucleosides)

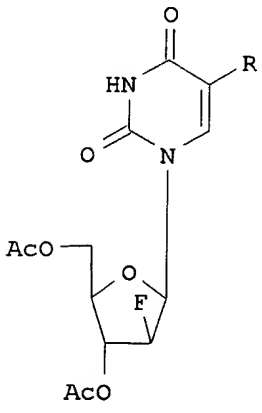
RN 134444-67-0 CAPLUS

CN 3'-Adenylic acid, 2'-deoxy-2'-fluoro-, 5'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 8 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1994:701206 CAPLUS
DOCUMENT NUMBER: 121:301206
TITLE: Derivatives of 1-(2-deoxy-2-fluoro-.beta.-D-arabinofuranosyl)-5-phenyluracil and 5-benzyluracil. Synthesis and biological properties
AUTHOR(S): Dziewiszek, Krzysztof; Schinazi, Raymond F.; Chou, Ting-Chao; Su, Tsann-Long; Dzik, Jolanta M.; Rode, Wojciech; Watanabe, Kyoichi A.
CORPORATE SOURCE: Mem. Sloan-Kettering Cancer Cent., Sloan-Kettering Inst. Cancer Res., New York, NY, 10021, USA
SOURCE: Nucleosides Nucleotides (1994), 13(1-3), 77-94
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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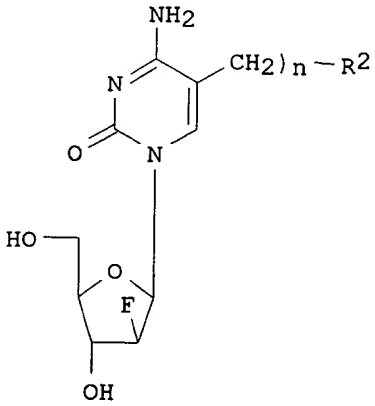


II

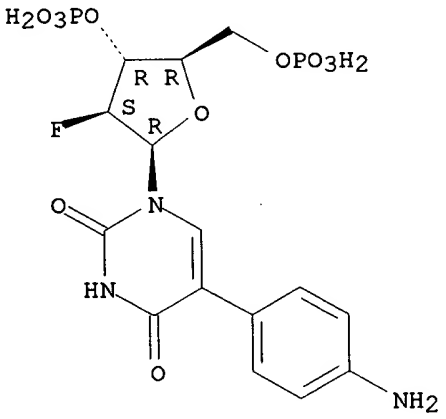
AB A no. of 1-(2-deoxy-2-fluoro-.beta.-arabinofuranosyl)uracil and -cytosine nucleosides, e.g. I (R = Ph, Bn) and II (R1 = C6H4NH2-2, C6H4NH2-4, n = 0, 1), were synthesized from 5-phenyl- and 5-benzyluracil via condensation of the fluorinated sugar, followed by nitration. The corresponding amino analogs were also prepd. by redn. of the nitro nucleosides. The uracil nucleosides were converted into the corresponding cytosine nucleosides by way of the triazole intermediates. None of these nucleosides exhibited

significant activity against herpes simplex virus type 1 in Vero cells. However, cytosine nucleosides contg. the .sigma.-nitrophenyl, p-nitrophenyl, p-nitrobenzyl or p-aminobenzyl substituent were found to be toxic (even at 1 .mu.M) to uninfected Vero cells, although they were essentially nontoxic in HL-60 cells. The 5'-monophosphates of the uracil nucleosides were inhibitors of the reaction catalyzed by purified Ehrlich ascites carcinoma thymidylate synthase, the 5-phenyluracil nucleotides causing a strong inhibition, competitive vs dUMP, described by the Ki value of 0.01 .mu.M.

IT **159042-52-1 159042-54-3 159042-60-1 159042-62-3 159042-65-6 159042-67-8 159042-69-0**
RL: RCT (Reactant)
(thymidylate synthase inhibition by)

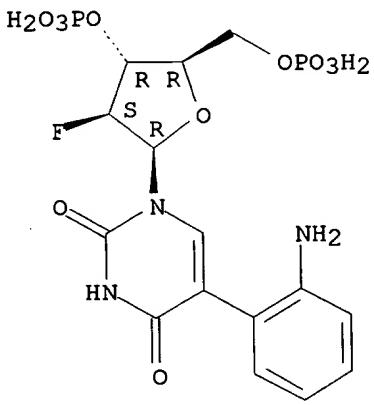
RN 159042-52-1 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-(4-aminophenyl)-1-(2-deoxy-2-fluoro-3,5-di-O-phosphono-.beta.-D-arabinofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



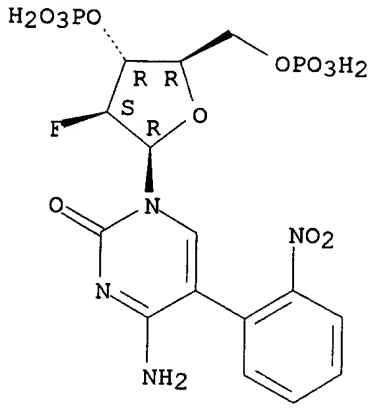
RN 159042-54-3 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-(2-aminophenyl)-1-(2-deoxy-2-fluoro-3,5-di-O-phosphono-.beta.-D-arabinofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



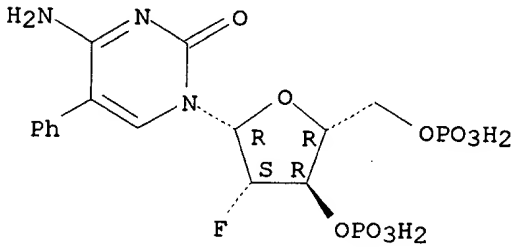
RN 159042-60-1 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-2-fluoro-3,5-di-O-phosphono-.beta.-D-arabinofuranosyl)-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



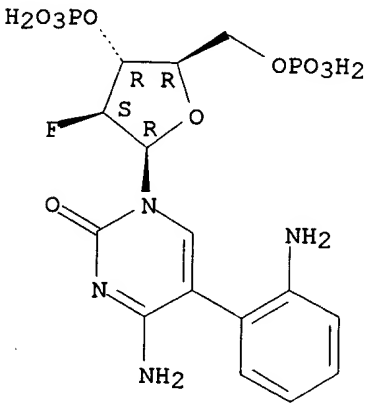
RN 159042-62-3 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-2-fluoro-3,5-di-O-phosphono-.beta.-D-arabinofuranosyl)-5-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159042-65-6 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-5-(2-aminophenyl)-1-(2-deoxy-2-fluoro-3,5-di-O-phosphono-.beta.-D-arabinofuranosyl)- (9CI) (CA INDEX NAME)

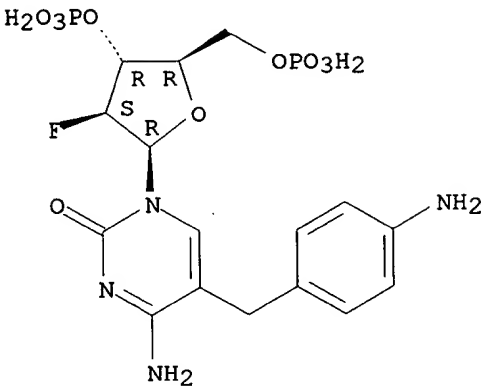
Absolute stereochemistry.



RN 159042-67-8 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-5-[(4-aminophenyl)methyl]-1-(2-deoxy-2-fluoro-3,5-di-O-phosphono-.beta.-D-arabinofuranosyl)- (9CI) (CA INDEX NAME)

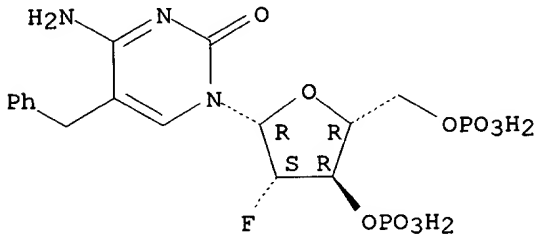
Searched by Barb O'Bryen, STIC 308-4291

Absolute stereochemistry.



RN 159042-69-0 CAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-(2-deoxy-2-fluoro-3,5-di-O-phosphono-.beta.-D-arabinofuranosyl)-5-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 9 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1994:509561 CAPLUS
DOCUMENT NUMBER: 121:109561
TITLE: Formation of triplexes of diastereoisomers of 2'-O-methyladenylyl-3',5'-2'-O-methyladenosine ethylphosphotriesters and 2'-O-methyladenylyl-3',5'-2'-O-methyladenosine methyl phosphonates with polyuridylic acid and polyuridylic acid and polythymidylic acid: a steric effect
AUTHOR(S): Kan, Lou Sing; Koo, William; Yano, Junichi
CORPORATE SOURCE: Inst. Chem., Acad. Sin., Taipei, Taiwan
SOURCE: J. Chin. Chem. Soc. (Taipei) (1993), 40(6), 631-6
CODEN: JCCTAC; ISSN: 0009-4536
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The triplex formation of diastereoisomers of 2'-O-methyladenylyl-3',5'-2'-O-methyladenosine ethylphosphotriesters and 2'-O-methyladenylyl-3',5'-2'-O-methyladenosine Me phosphonates with polyuridylic acid and polythymidylic acid was monitored by UV spectral methods. Possible steric effects on the stability of the triplex are discussed with the aid of simulated chem. structures.

IT **155180-26-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and melting temp. of)

RN 155180-26-0 CAPLUS
CN 5'-Uridylic acid, homopolymer, complex with 2'-O-methyladenylyl-

(3'.fwdarw.5')-2'-O-methyladenosine (2:1) (9CI) (CA INDEX NAME)

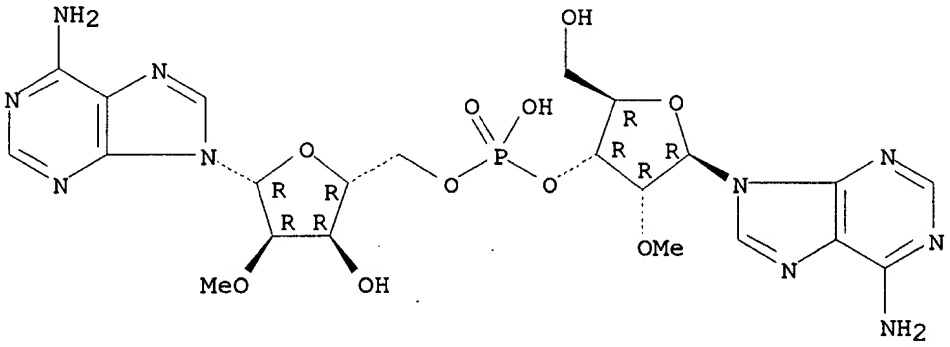
CM 1

CRN 155180-25-9
CMF C22 H29 N10 O10 P . (C9 H13 N2 O9 P)x

CM 2

CRN 54621-66-8
CMF C22 H29 N10 O10 P
CDES 5:B-D-RIBO,B-D-RIBO

Absolute stereochemistry.



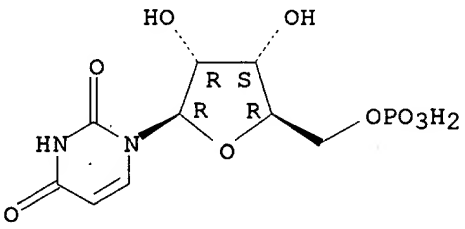
CM 3

CRN 27416-86-0
CMF (C9 H13 N2 O9 P)x
CCI PMS

CM 4

CRN 58-97-9
CMF C9 H13 N2 O9 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



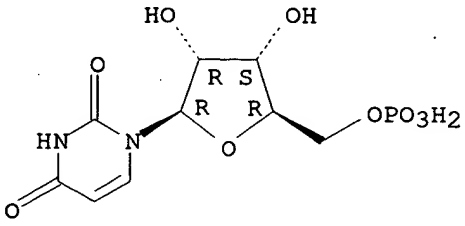
CM 5

CRN 27416-86-0
CMF (C9 H13 N2 O9 P)x
CCI PMS

CM 6

CRN 58-97-9
CMF C9 H13 N2 O9 P
CDES 5:B-D-RIBO

Absolute stereochemistry.

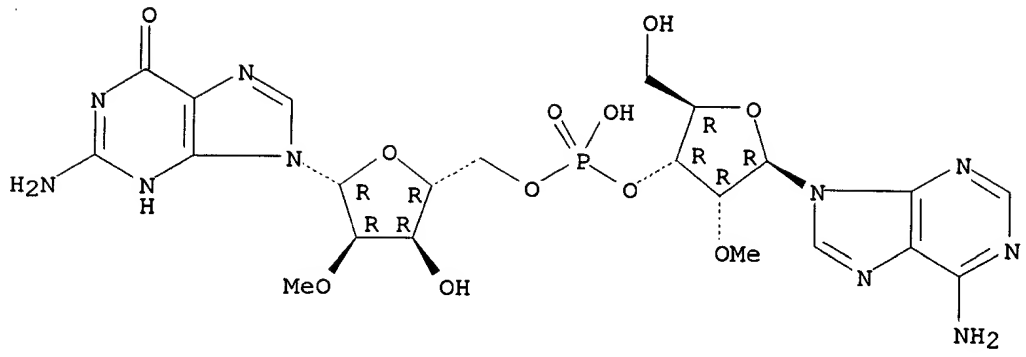


L51 ANSWER 10 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1992:401889 CAPLUS
DOCUMENT NUMBER: 117:1889
TITLE: Initiator oligonucleotides for the combination of chemical and enzymic RNA synthesis
AUTHOR(S): Pitulle, Christian; Kleineidam, Reinhard G.; Sproat, Brian; Krupp, Guido
CORPORATE SOURCE: Inst. Allg. Mikrobiol., Christian-Albrechts-Univ., Kiel, W-2300, Germany
SOURCE: Gene (1992), 112(1), 101-5
CODEN: GENED6; ISSN: 0378-1119
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Transcription reactions with T7 RNA polymerase were performed in the presence of short oligonucleotides (oligos) with guanosine at the 3'-end. Transcripts were obtained which had included these initiator oligos at their 5'-termini. The oligos could contain mixts. of deoxyribo-, ribo-, 2'-O-methylated and biotinylated nucleotides. Only the 3'-terminal guanosine of these oligos was encoded in the template DNA at the transcription start point, in contrast to the remainder of the sequence. This 5'-terminal sequence is variable and eliminates the limitation that transcripts must start with a 5'-terminal guanosine. With a 5'-biotinylated dinucleotide, end-labeled RNAs were obtained which are suitable for nonradioactive RNA sequencing.

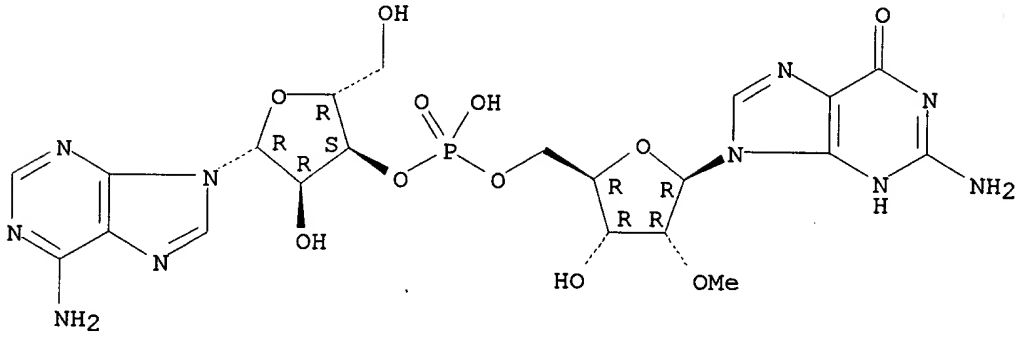
IT **54621-67-9P 142783-36-6P**
RL: PREP (Preparation)
(prepn. of and T7 RNA polymerase-mediated transcription initiation by, nonradioactive RNA sequencing in relation to)
RN 54621-67-9 CAPLUS
CN Guanosine, 2'-O-methyladenylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 142783-36-6 CAPLUS
CN Guanosine, adenylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 11 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1991:630514 CAPLUS
DOCUMENT NUMBER: 115:230514
TITLE: Preparation of 2'-deoxy-2'-fluororibonucleosides as medicinal virucides
INVENTOR(S): Tisdale, Sylvia Margaret; Van Tuttle, Joel; Slater, Martin John; Daluge, Susan Mary; Miller, Wayne Howard; Krenitsky, Thomas Anthony; Koszalka, George Walter
PATENT ASSIGNEE(S): Wellcome Foundation Ltd., UK
SOURCE: Eur. Pat. Appl., 44 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

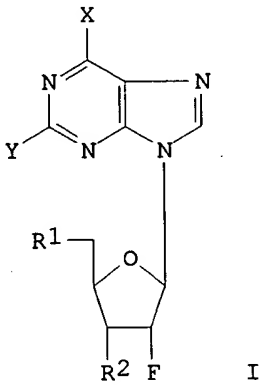
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 417999	A1	19910320	EP 1990-309838	19900907
EP 417999	B1	19960313		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DD 297650	A5	19920116	DD 1990-343871	19900907
EP 671410	A1	19950913	EP 1995-107762	19900907
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 135365	E	19960315	AT 1990-309838	19900907
CA 2025009	AA	19910312	CA 1990-2025009	19900910
AU 9062350	A1	19910314	AU 1990-62350	19900910

Searched by Barb O'Bryen, STIC 308-4291

AU 644095	B2	19931202			
HU 54704	A2	19910328	HU 1990-5841	19900910	
ZA 9007187	A	19920527	ZA 1990-7187	19900910	
PL 164967	B1	19941031	PL 1990-286820	19900910	
RU 2043361	C1	19950910	RU 1990-4831211	19900910	
JP 03145497	A2	19910620	JP 1990-241057	19900911	
PRIORITY APPLN. INFO.:			GB 1989-20534	19890911	
			EP 1990-309838	19900907	

OTHER SOURCE(S): MARPAT 115:230514

GI



I

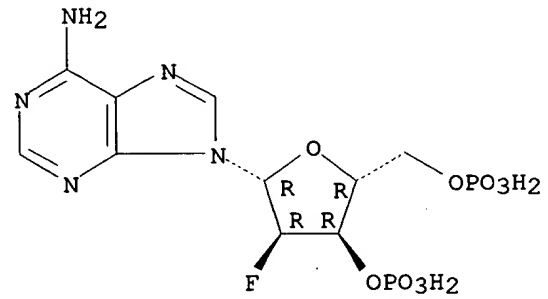
AB 2'-Deoxy-2'-fluororibonucleosides I [Y = H, NH2; X = (substituted) amino, ZR3; Z = O, S; R1,R2 = OH, OCOR4H, H, OCO2R5H, etc.; R3 = (substituted) C1-6 alkenyl, or C3-7 cycloalkyl; R4 = (hydroxy) C1-6 alkylene, C2-6 alkenylene, or C3-7 cycloalkylene; R5 = bond, R4] were prepd. For example, 2-amino-6-methoxypurine and 1-(2-deoxy-2-fluoro-.beta.-D-ribofuranosyl)uracil were converted to title compd. I (R1 = R2 = OH, X = OMe, Y = NH2) (II) by thymidine phosphorylase and purine nucleoside phosphorylase in potassium phosphate buffer contg. potassium azide. The IC50 of II against respiratory syncytial virus was 6.3 .mu.M. Formulations of I were prepd.

IT **134444-67-0P**
RL: PREP (Preparation)
(prepn. of, as antiviral agent)

RN 134444-67-0 CAPLUS

CN 3'-Adenylic acid, 2'-deoxy-2'-fluoro-, 5'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



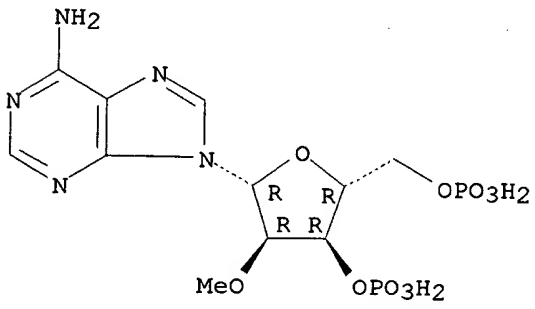
Searched by Barb O'Bryen, STIC 308-4291

L51 ANSWER 12 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1988:2419 CAPLUS
DOCUMENT NUMBER: 108:2419
TITLE: Role of a bulged A residue in a specific RNA-protein interaction
AUTHOR(S): Wu, Huey Nan; Uhlenbeck, Olke C.
CORPORATE SOURCE: Dep. Chem. Biochem., Univ. Colorado, Boulder, CO, 80309, USA
SOURCE: Biochemistry (1987), 26(25), 8221-7
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The translational operator of the RNA replicase gene of phage R17 contains a bulged adenylyl (A) residue that is essential for the specific binding to R17 coat protein. A large no. of operator variants were synthesized to more precisely examine the role of the bulged A residue on this specific protein-RNA interaction. By use of RNA ligase and transcription of synthetic DNA templates by T7 RNA polymerase, 14 different nucleotides were introduced to the bulged A position of 3 different coat protein-binding fragments. The affinity between the coat protein and each fragment was detd. by a nitrocellulose filter binding assay. The data indicated that whereas functional groups on N1, O2, C6, N7, and 2'OH of the bulged A could be substituted without greatly changing protein binding, bulky substituents could not be tolerated at these positions. Data from addnl. fragments that have base-pair changes adjacent to the bulged A suggested that the propensity of the bulged A to intercalate into the helix can affect protein binding.

IT **54619-24-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with oligonucleotides)
RN 54619-24-8 CAPLUS
CN 3'-Adenylic acid, 2'-O-methyl-, 5'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

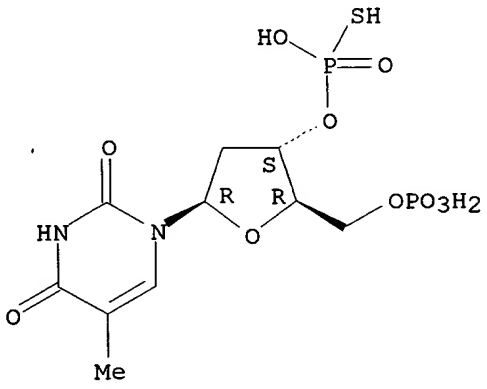
Absolute stereochemistry.



L51 ANSWER 13 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1985:2856 CAPLUS
DOCUMENT NUMBER: 102:2856
TITLE: Use of 2'-deoxy-5'-phosphothymidine 3'-phosphothioate in a reaction catalyzed by T4 phage RNA-ligase - route to 3'-substituted oligoribonucleotides. Derivative with the 3'-terminal function that can be switched on
AUTHOR(S): Oshevskii, S. I.; Bogachev, V. S.; Kumarev, V. P.
CORPORATE SOURCE: Inst. Cytol. Genet., Novosibirsk, USSR
SOURCE: Bioorg. Khim. (1984), 10(9), 1190-8
Searched by Barb O'Bryen, STIC 308-4291

CODEN: BIKHD7
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The prepn. of 2'-deoxy-5'-phosphothymidine 3'-phosphothioate (I), based on the modified method for the synthesis of nucleoside-3'-phosphothioates (Chladek, S.; Nagyvary, J., 1972), involves treatment of 5'-protected nucleoside deriv. with PSCl3 in pyridine (5.degree.). Incubation of I with oligoribonucleoside (Ap)5A at 37.degree. for 1 h in the presence of T4 phase RNA ligase gave mixed oligoribo(deoxyribo)nucleoside (Ap6)dTps. Alkylation of this nucleoside (32 .mu.M) with N-methyl-N,N'-di-(2-chloroethyl)-N'-(p-formylphenyl)trimethylenediamine (700 .mu.M) yielded the monoalkylated product (>95%). The formyl group of the 5-alkyl deriv., which contained an intact 2-chloroethylamino group at the 3'-end of the oligonucleotide, was reduced with 1M NaBH4 under mild conditions (0.05M borate buffer pH 8.3) to activate the 2-chloroethylamino group. Such oligonucleotide reagents are suitable for addressed chem. modification of nucleic acids and proteins.
IT **93464-27-8P**
RL: PREP (Preparation)
(prepn. and oligonucleotide reaction with)
RN 93464-27-8 CAPLUS
CN 5'-Thymidylic acid, 3'-(dihydrogen phosphorothioate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 14 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1984:434658 CAPLUS
DOCUMENT NUMBER: 101:34658
TITLE: Chemical synthesis of the 5'-terminal part bearing cap structure of messenger RMA of cytoplasmic polyhedrosis virus (CPV): m7G5'pppAmpG and m7G5'pppAmpGpU
AUTHOR(S): Yamaguchi, Kazuo; Nakagawa, Iwao; Sekine, Mitsuo; Hata, Tsujiaki; Shimotohno, Kunitada; Hiruta, Michiyo; Miura, Kinichiro
CORPORATE SOURCE: Dep. Life Chem., Tokyo Inst. Technol., Yokohama, 227, Japan
SOURCE: Nucleic Acids Res. (1984), 12(6), 2939-54
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

Searched by Barb O'Bryen, STIC 308-4291

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The 5'-terminal cap structures of mRNA of CPV, m7G5ppmAmpG and m7G5ppmAmpGpU (I) were chem. synthesized. S,S-Di(4-methoxyphenyl)-N6-benzoyl-2'-O-methyladenosine 5'-phosphorodithioate [(ArS)2pAmbz)6] was prepd. by phosphorylation of the 5'-OH group of N6-benzoyl-2'-O-methyladenosine with S,S-di(4-methoxyphenyl)phosphorodithioate by cyclohexylammonium S,S-bis(4-methoxyphenyl)phosphorodithiolate. By the triester approach using (ArS)2pAmbz as starting material, the protected dinucleotide and trinucleotide bearing the 5'-phosphate group were synthesized. The protective groups of the dinucleotide and trinucleotide were removed to obtain pAmpG and pAmpGpU, resp. By the reaction of a capping agent (P1-S-phenyl-P2-7-methylguanosine 5'-pyrophosphorothiolate) with pAmpG and pAmpGpU in the presence of AgNO3 or I2. The 5'-terminal structure of the mRNA strand of CPV, which was labeled isotopically, was confirmed completely as I by cochromatotog. with the synthesized nucleotides.

IT **90735-35-6**
RL: RCT (Reactant)
(reaction of, with phenylmethylguanosine pyrophorphorothiolate salt)

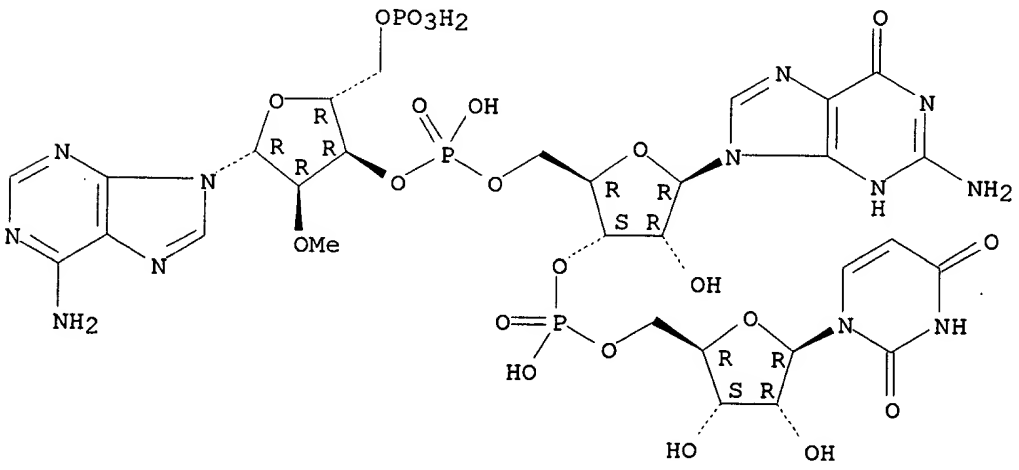
RN 90735-35-6 CAPLUS

CN Uridine, 2'-O-methyl-5'-O-phosphonoadenylyl-(3'.fwdarw.5')-guanylyl-(3'.fwdarw.5')-, compd. with N,N-dibutyl-1-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 90735-34-5
CMF C30 H39 N12 O22 P3
CDES 5:B-D-RIBO,B-D-RIBO,B-D-RIBO

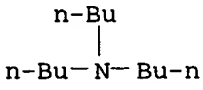
Absolute stereochemistry.



CM 2

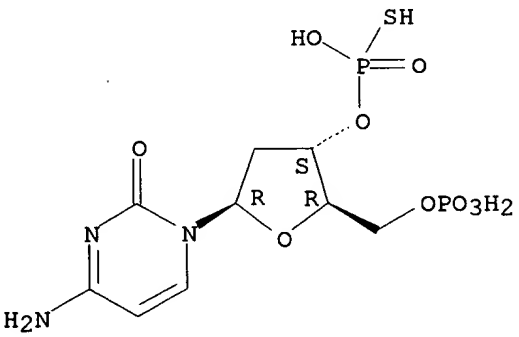
CRN 102-82-9
CMF C12 H27 N

Searched by Barb O'Bryen, STIC 308-4291



L51 ANSWER 15 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1984:205881 CAPLUS
DOCUMENT NUMBER: 100:205881
TITLE: Fluorescent labeling of tRNA and oligodeoxynucleotides using T4 RNA ligase
AUTHOR(S): Cosstick, Richard; McLaughlin, Larry W.; Eckstein, Fritz
CORPORATE SOURCE: Abt. Chem., Max-Planck-Inst. Exp. Med., Goettingen, D-3400, Fed. Rep. Ger.
SOURCE: Nucleic Acids Res. (1984), 12(4), 1791-810
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 3'-O-(5'-Phosphoryldeoxycytidyl) phosphorothioate and fluorescent 3'-O-(5'-phosphoryldeoxycytidyl) S-bimane phosphorothioate can be ligated to tRNA by T4 RNA ligase. They are also efficient donors for the enzymic ligation to oligodeoxynucleotides bearing a 3'-cytidine terminus. Cytidine 3',5'-bisphosphate is also a substrate for the ligation reaction with DNA restriction fragments with a 3'-terminal cytidylic acid residue. Oligo- and polynucleotides with a 3'-phosphorothioate group react readily with electrophiles as exemplified by the reaction with monobromobimane.
IT **90293-67-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with monobromobimane)
RN 90293-67-7 CAPLUS
CN 5'-Cytidylic acid, 2'-deoxy-, 3'-(dihydrogen phosphorothioate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 16 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1983:517980 CAPLUS
DOCUMENT NUMBER: 99:117980
TITLE: Intramolecular stacking association and conformation properties of a cap structure, m7G5'pppUm, and the related model compounds
AUTHOR(S): Tazawa, Ichiro; Inoue, Yasuo
CORPORATE SOURCE: Fac. Sci., Univ. Tokyo, Hongo, 113, Japan
SOURCE: Nucleic Acids Res. (1983), 11(9), 2907-15
CODEN: NARHAD; ISSN: 0305-1048
Searched by Barb O'Bryen, STIC 308-4291

DOCUMENT TYPE: Journal
LANGUAGE: English

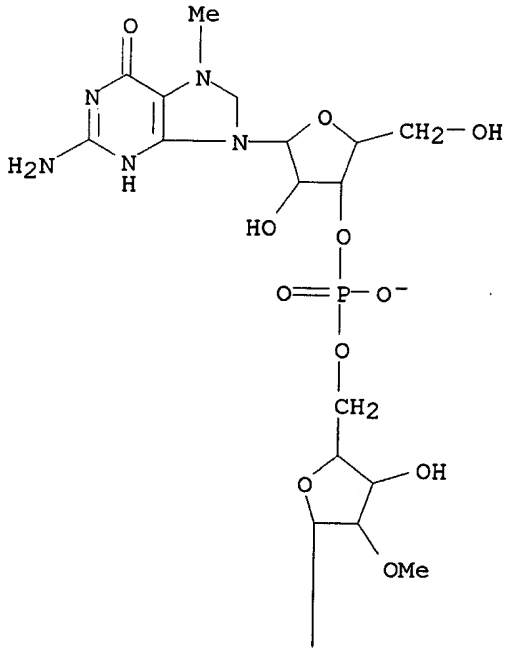
AB The stacking equil. quotient of the m7G5'pppUm (where m7G is 7-methylguanosine and Um is 2'-O-methyluridine) unit, which occurs as the 5'-terminal cap of certain eukaryotic mRNA's, was detd. by temp.-dependent difference spectrophotometry as Kstack = 1.82 at 25.degree. and pH 5. To evaluate the contribution of different structural modifications to the net stabilization of the cap structures of mRNA, a variety of compds. related to m7G5'pppUm were synthesized and their stacking properties were studied by the same method and compared. Introduction of a Me group into N-7 of guanosine (G) residue results in an increase in base stacking. Methylation at 2'-OH or uridine residue also stabilizes the stacked structure of G-contg. dimers, but it does not influence stacking interaction in m7G-contg. dimers. The effect of different types of internucleotide linkages on the order of stacking tendencies is: N5'PPN' > N5'pppN' > NpN' (where N is an undefined nucleoside). UV hypochromicity and CD spectral measurements of the relevant dimers were also conducted, and the hypochromicity values and CD spectra of dimers in their stacked conformation were estd. by making use of the detd. Kstack values. Whereas 2'-O-methylation exerts very little effect on the stacked conformation of the dimers, methylation at N-7 and the nature of the internucleotide linkage strongly influence the stacked conformation, thereby forming unusual left-handed conformations in m7G5'pppU(m), m7G5'ppU(m), and G5'ppU(m).

IT **84609-36-9 84626-09-5**
RL: BIOL (Biological study)
(stacking assocn. and conformational properties of)

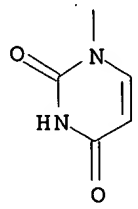
RN 84609-36-9 CAPLUS

CN 5'-Uridylic acid, 2'-O-methyl-, 5'.fwdarw.3'-ester with 2-amino-6,9-dihydro-7-methyl-6-oxo-9-.beta.-D-ribofuranosyl-1H-purinium, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A

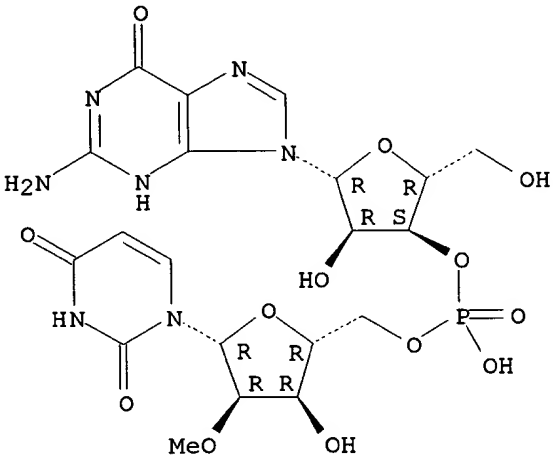


PAGE 2-A



*** FRAGMENT DIAGRAM IS INCOMPLETE ***
RN 84626-09-5 CAPLUS
CN Guanosine, 2'-O-methyluridylyl-(5'.fwdarw.3')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L51 ANSWER 17 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1983:85003 CAPLUS
DOCUMENT NUMBER: 98:85003
TITLE: Chemical synthesis and intramolecular association studies of a cap structure, m7G5'pppUm, and the related model compounds
AUTHOR(S): Tazawa, Ichiro; Inoue, Yasuo
CORPORATE SOURCE: Fac. Sci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Nucleic Acids Symp. Ser. (1982), 11(Symp. Nucleic Acids Chem., 10th, 1982), 257-60
CODEN: NACSD8; ISSN: 0261-3166
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The stacking equil. quotient of the m7G5'pppUm component, which occurs as the 5'-terminal cap of certain eukaryotic mRNAs, was detd. by temp.-dependent difference spectrophotometry to be 1.82 at 25.degree., pH 5. To evaluate the contribution of different structural modifications to stabilizing the cap structures of mRNA, a variety of compds. related to m7G5'pppUm were synthesized and their stacking properties were studied by the same method and compared. The introduction of a Me group into the guanine base (at N-7) results in an increase in base stacking. Me substitution at 2'-OH also stabilizes the stacked structure, but this effect is less pronounced than the N-7 methylation of the guanine residue. The effect of different types of internucleotide linkage on the order of stacking tendencies is N5'ppN' > N5'pppN' > N3'pN'.

IT **84609-36-9 84626-09-5**

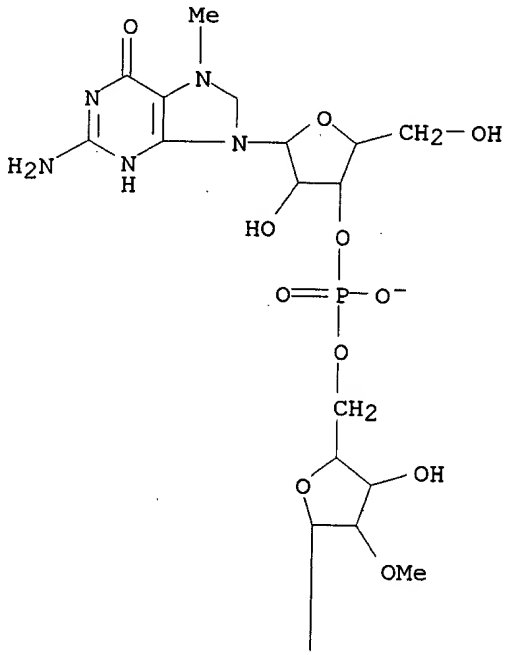
Searched by Barb O'Bryen, STIC 308-4291

RL: BIOL (Biological study)
(stacking in, mRNA cap structure in relation to)

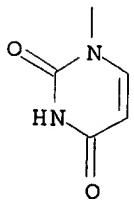
RN 84609-36-9 CAPLUS

CN 5'-Uridylic acid, 2'-O-methyl-, 5'.fwdarw.3'-ester with 2-amino-6,9-dihydro-7-methyl-6-oxo-9-.beta.-D-ribofuranosyl-1H-purinium, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

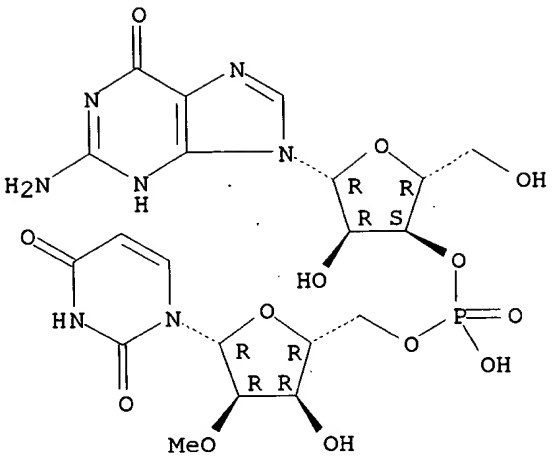


*** FRAGMENT DIAGRAM IS INCOMPLETE ***

RN 84626-09-5 CAPLUS

CN Guanosine, 2'-O-methyluridylyl-(5'.fwdarw.3')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

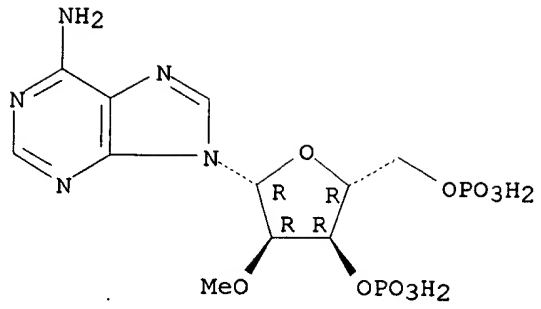


L51 ANSWER 18 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1982:468012 CAPLUS
DOCUMENT NUMBER: 97:68012
TITLE: Modified nucleotides: their conformational characteristics
AUTHOR(S): Ponnuswamy, P. K.; Anukanth, A.
CORPORATE SOURCE: Auton. Postgrad. Cent., Univ. Madras, Tamilnadu, 620 020, India
SOURCE: J. Theor. Biol. (1982), 96(2), 233-51
CODEN: JTBIAP; ISSN: 0022-5193
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Potential energy as contributions from nonbonded, electrostatic, H bonding, and torsional interactions was computed as a function of dihedral angles around the glycosyl and exocyclic bonds for 4 important modified nucleic acid subunits, viz. pseudouridine with an unusual glycosyl bond, dihydrouridine with a satd. base ring, N,N'-dimethylguanosine having double methylation in the base ring, and 2'-O-methyladenosine having methylation in the ribose moiety. The 2 preferred, C2-endo and C3-endo, sugar puckers were considered. The probable low energy regions in the .chi.-.psi. space and the population of various conformational states for each of the mols. were detd. The results of modified units were compared with those of the corresponding normal units. Exptl. results available on simple mol. systems and on tRNA mols. were used for comparisons with theor. predictions.

IT **54619-24-8**
RL: PRP (Properties)
(conformational forms and potential energy of)
RN 54619-24-8 CAPLUS
CN 3'-Adenylic acid, 2'-O-methyl-, 5'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

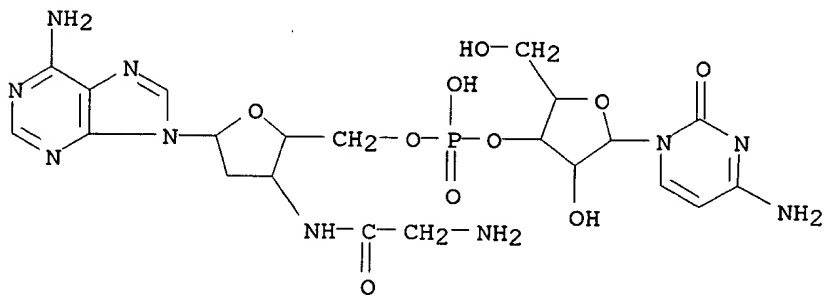


L51 ANSWER 19 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1979:99135 CAPLUS
DOCUMENT NUMBER: 90:99135
TITLE: Stereochemical control of the ribosomal peptidyltransferase reaction. The role of acceptor substrate amino acid side chain orientation
AUTHOR(S): Bhuta, Aruna; Chladek, Stanislav
CORPORATE SOURCE: Michigan Cancer Found., Detroit, Mich., USA
SOURCE: FEBS Lett. (1978), 96(1), 23-5
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several 2'(3')-aminoacyloligonucleotides were used as analogs of 2'- and 3'-aminoacyl-tRNA acceptor termini in the peptidyltransferase reaction using the fMet-tRNA.cntdot.A-U-G.cntdot.70S ribosome system. The 3'-isomer, C-2'-dA-Phe was more active than the 2'-isomer, C-3'-dA-Phe, the apparent Km ratio being >2 orders of magnitude. The 3'-ester, C-2'-dA-Leu was a far more preferable acceptor of the fMet residue relative to the practically inactive C-3'-dA-Leu. However, C-2'-dA-Gly, C-3'-dA-Gly, C-3'-NH2A-Gly, and C-2'-NH2A-Gly displayed comparable activities, with the 3'-derivs. being only slightly preferred (apparent Km ratio (2'/3') .apprx.2). Thus, the peptidyltransferase A site is probably specific for 3'-aminoacyl acceptors derived from optically active amino acids, whereas there is virtually no specificity for 2'- and 3'-glycyl derivs.

IT **69319-90-0**
RL: BIOL (Biological study)
(as peptidyltransferase acceptor substrate, stereospecificity for)

RN 69319-90-0 CAPLUS
CN Adenosine, cytidylyl-(3'.fwdarw.5')-3'-[(aminoacetyl)amino]-2',3'-dideoxy-(9CI) (CA INDEX NAME)



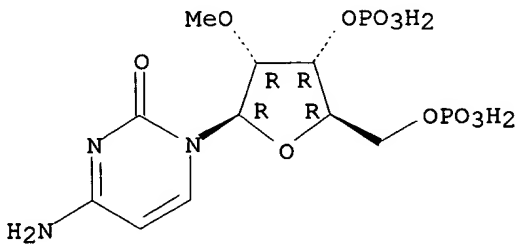
Searched by Barb O'Bryen, STIC 308-4291

L51 ANSWER 20 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1978:611011 CAPLUS
DOCUMENT NUMBER: 89:211011
TITLE: Synthesis of modified nucleoside 3',5'-bisphosphates and their incorporation into oligoribonucleotides with T4 RNA ligase
AUTHOR(S): Barrio, Jorge R.; Barrio, Maria del Carmen G.; Leonard, Nelson J.; England, Thomas E.; Uhlenbeck, Olke C.
CORPORATE SOURCE: Sch. Chem. Sci., Univ. Illinois, Urbana, Ill., USA
SOURCE: Biochemistry (1978), 17(11), 2077-81
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A simple procedure is described to prep. nucleoside 3'(2'),5'-diphosphates from the corresponding nucleosides with the use of pyrophosphoryl chloride. This method is rapid, gives nearly quant. yields and, most importantly, can be used for a variety of nucleosides with base and sugar modifications. Since 3',5'-diphosphates are donors in the phage T4 RNA ligase reaction, a single residue can be enzymically attached to the 3'-end of oligoribonucleotides. By these procedures, 5 different ring-modified nucleosides and 1 sugar-modified nucleoside were incorporated onto the 3'-end of (Ap)3C. In 2 cases, an addnl. step of synthesis with RNA ligase resulted in the modified nucleotide being located in an internal position in the oligonucleotide. Thus, a general method for the synthesis of oligoribonucleotides contg. modified nucleosides is outlined. Since many of the modified nucleosides are fluorescent, oligomers contg. them should be useful in a variety of phys. and biochem. studies.

IT **67126-61-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and oligoribonucleotide enzymic formation from)
RN 67126-61-8 CAPLUS
CN 3'-Cytidylic acid, 2'-O-methyl-, 5'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

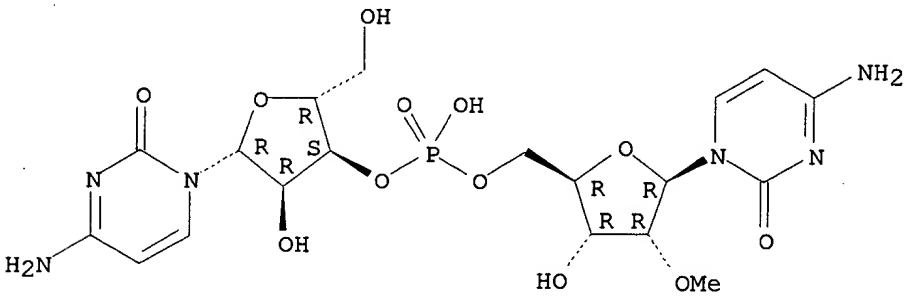
Absolute stereochemistry.



L51 ANSWER 21 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1978:121611 CAPLUS
DOCUMENT NUMBER: 88:121611
TITLE: Oligonucleotidic compounds. LXII. Synthesis of cytidylyl(3' .fwdarw. 5')-2'-O(and 3'-O)-methyladenosine 3'-O(and 2'-O)-N-formyl-L-methionyl derivatives
AUTHOR(S): Alexandrova, L. A.; Smrt, Jiri
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, Czech.
SOURCE: Collect. Czech. Chem. Commun. (1977), 42(5), 1694-1704
Searched by Barb O'Bryen, STIC 308-4291

CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Cytidylyl-(3'.fwdarw.5')-2'-O-methyl-3'-O-(N-formyl-L-methionyl)adenosine and cytidylyl-(3'.fwdarw.5')-2'-O-(N-formyl-L-methionyl)-3'-O-methyladenosine were prepd. by the action of N-formyl-L-methionylimidazole on 5'-O-[bis(p-methoxyphenyl)phenylmethyl]-2'-O-tetrahydropyranyl-N4-dimethylaminomethylenecytidylyl-(3'.fwdarw.5')-2'-O(and 3'-O, resp.)-methyl-N6-dimethylaminomethyleneadenosine followed by a stepwise removal of acid labile protecting groups. Contrary to dicyclohexylcarbodiimide, 1-(p-tolylsulfonyl)-1,2,4-triazole in C5H5N did not racemize N-formyl-L-methionine in the reaction with 5'-O-[bis(p-methoxyphenyl)phenylmethyl]-2'-O-methyl-N6-dimethylaminomethyleneadenosine to 5'-O-[bis(p-methoxyphenyl)phenylmethyl]-2'-O-methyl-3'-O-(N-formyl-L-methionyl)-N6-dimethylaminomethyleneadenosine .
IT **65798-46-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 65798-46-1 CAPLUS
CN Cytidine, cytidylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



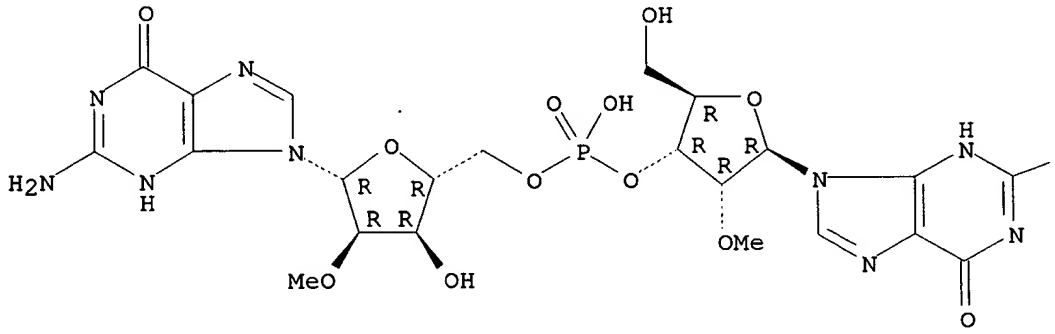
L51 ANSWER 22 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1977:463453 CAPLUS
DOCUMENT NUMBER: 87:63453
TITLE: Effects of a trinucleotide ethyl phosphotriester, Gmp(Et)Gmp(Et)U, on mammalian cells in culture
AUTHOR(S): Miller, Paul S.; Braiterman, Lita T.; Ts'o, Paul O. P.
CORPORATE SOURCE: Sch. Hyg. Public Health, Johns Hopkins Univ., Baltimore, Md., USA
SOURCE: Biochemistry (1977), 16(9), 1988-96
CODEN: BICHAW
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The nonionic 2'-O-methylribooligonucleotide ethyl phosphotriester Gmp(Et)Gmp(Et)U (I) [63224-55-5] was synthesized and shown to be complementary to base sequences found in most tRNA and some mRNA mols. I treatment of a culture of transformed fibroblasts inhibited cellular protein synthesis and slightly increased RNA synthesis, but macromol. formation returned toward normal after 4 h. I or its deethylated metabolities may act by phys. binding to tRNA and mRNA, thus inhibiting their functions. The reversible inhibition of protein synthesis could reflect a further degrdn. of the trinucleotide or an increase in the supply of RNA mols. involved in protein synthesis. I caused a temporary decrease in the rate of fibroblast growth during the first 24 h, and decreased the no. and size of colonies formed by thr transformed fibroblasts.

Searched by Barb O'Bryen, STIC 308-4291

IT **63224-54-4P**
RL: PREP (Preparation)
(prepn. of)
RN 63224-54-4 CAPLUS
CN Guanosine, 2'-O-methylguanylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

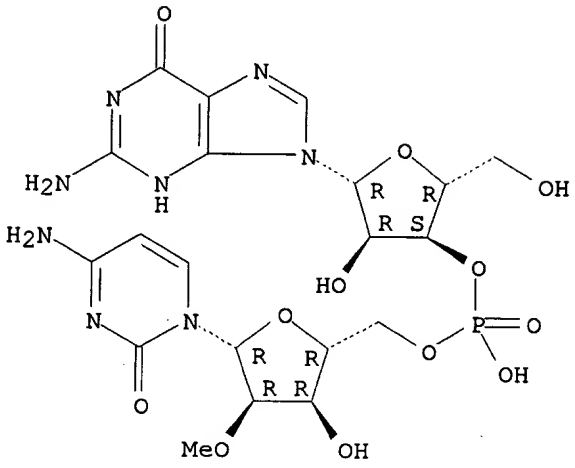


PAGE 1-B

—NH2

L51 ANSWER 23 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1977:30024 CAPLUS
DOCUMENT NUMBER: 86:30024
TITLE: Oligoribonucleotide synthesis. X. An improved synthesis of the anticodon loop region of methionine transfer ribonucleic acid from E. coli
AUTHOR(S): Werstiuk, E. S.; Neilson, Thomas
CORPORATE SOURCE: Dep. Biochem., McMaster Univ., Hamilton, Ont., Can.
SOURCE: Can. J. Chem. (1976), 54(17), 2689-96
CODEN: CJCHAG
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nonaribonucleotide, GpCmpUpCpApUpApApC, (m = 2'-O-methyl) was synthesized using a block phosphotriester method. Its sequence corresponds to that of the anticodon loop of transfer RNAfMet. Protected tetramer, GCmUC and pentamer nucleotides, AUAAC, assembled stepwise from nucleoside derivs., were joined together to give protected nonamer which on deblocking, gave the free nonaribonucleotide. The superior internucleotide coupling efficiency of mesitylenesulfonyl triazolide over triisopropylbenzenesulfonyl chloride is demonstrated.
IT **52571-48-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 52571-48-9 CAPLUS
CN Guanosine, 2'-O-methylcytidylyl-(5'.fwdarw.3')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



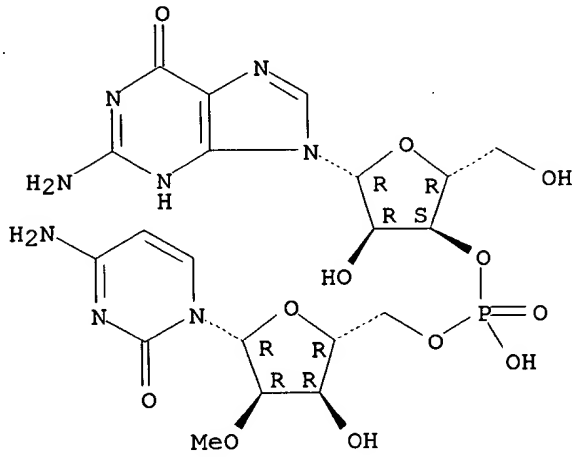
L51 ANSWER 24 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1976:572945 CAPLUS
DOCUMENT NUMBER: 85:172945
TITLE: Influence of ribose 2'-O-methylation on GpC conformation by classical potential energy calculations
AUTHOR(S): Stellman, Steven D.; Broyde, Suse B.; Wartell, Roger M.
CORPORATE SOURCE: Am. Health Found., New York, N. Y., USA
SOURCE: Biopolymers (1976), 15(10), 1951-64
CODEN: BIPMAA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Potential energy calcns. were employed to exam. the effect of ribose 2'-O-methylation on the conformation of GpC. Min. energy conformations and allowed conformational regions were calcd. for 2'-O-methyl-GpC (2'MeGpC) and Gp-2'-O-methyl-C (Gp2'MeC). The 2 lowest energy conformations of 2'MeGpC and Gp2'MeC are similar to those of GpC itself. The helical RNA conformation (sugar pucker-C(3')-endo,.omega.' and .omega.,g-g-, bases-anti) is the global min., and a helix-reversing conformation with .omega.',.omega. in the vicinity of 20.degree., 80.degree. is next in energy. However, subtle differences between the 3 mols. were noted. When the substitution is on the 5' ribose (Gp2'MeC), the energy of the helical conformation is less than that of GpC, due to favorable interactions of the added Me group. When the substitution is at the 3' ribose (2'MeGpC) these stabilizing interactions are outweighed by steric restrictions, and the helical conformation is of higher energy than for GpC. Furthermore, the statistical wt. of the 2'MeGpC g-g- helical region is substantially less than the corresponding wt. for Gp2'MeC. In addn., the 2'MeGpC methoxy group is conformationally restricted to a narrow range centered at 76.degree.. This group has a broadly allowed region between 50 and 175.degree. in Gp2'MeC. These differences occur because the appended Me group in 2'MeGpC is located in the interior of the helix cylinder, whereas it hangs unimpeded in Gp2'MeC. These findings suggested that 2'-O-methylation has both stabilizing and destabilizing influences on the helical conformation of RNA. For 2'MeGpC the destabilizing steric hindrance imposed by the nature of the guanine base dominates.

IT **52571-48-9**
RL: PRP (Properties)
(conformation of, methyl group in relation to)

RN 52571-48-9 CAPLUS
CN Guanosine, 2'-O-methylcytidylyl-(5'.fwdarw.3')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

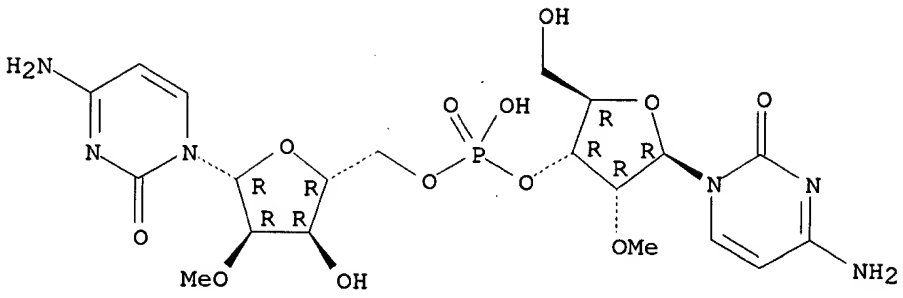


L51 ANSWER 25 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1976:555217 CAPLUS
DOCUMENT NUMBER: 85:155217
TITLE: Dinucleoside monophosphates. II. Nearest neighbor interactions
AUTHOR(S): Topal, Michael D.; Warshaw, Myron M.
CORPORATE SOURCE: Dep. Chem., New York Univ., New York, N. Y., USA
SOURCE: Biopolymers (1976), 15(9), 1775-93
CODEN: BIPMAA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A method was developed which enabled calcn. and unambiguous comparison of the thermodn. for the stacking process of dinucleoside monophosphates (dimers) from a study of their titrn. properties. This method was applied to dimers contg. adenosine and(or) cytidine, with the result that the dimers studied were ordered with respect to their tendency to stack as ApA > ApC > CpA .simeq. C-contg. homodimers. This dependence of the relative magnitude of .DELTA.Fstacking on compn. is consistent with hydrophobic interactions being the main driving force toward stacking. The sequence dependence of .DELTA.Fstacking as well as of the optical properties of the dimers is related to van der Waals interaction between the bases. The lack of variation in .DELTA.Fstacking of the C-contg. isomers indicated that the role of the 2'-OH in RNA vs. DNA structure is not H bonding.

IT **60731-39-7**
RL: BIOL (Biological study)
(stacking interactions of, thermodn. of, hydrophobicity in relation to)
RN 60731-39-7 CAPLUS
CN Cytidine, 2'-O-methylcytidylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

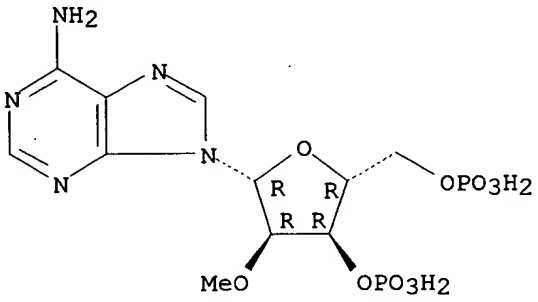


L51 ANSWER 26 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1975:58049 CAPLUS
DOCUMENT NUMBER: 82:58049
TITLE: Effect of ribose O(2')-methylation on the conformation of nucleosides and nucleotides
AUTHOR(S): Prusiner, P.; Yathindra, N.; Sundaralingam, M.
CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, Wis., USA
SOURCE: Biochim. Biophys. Acta (1974), 366(2), 115-23
CODEN: BBACAQ
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Semi-empirical conformational energy calcns. using partitioned functions were done on 2'-O-methyladenosine, the corresponding 5'-nucleotide and the 3',5'-diphosphate to assess the influence of the 2'-methoxy group on their favored conformations. Calcns. were done for the two modes of sugar puckerings obsd. in the crystal structure of 2'-O-methyladenosine, C-3'-endo-C-2'-exo, 3T2, and C-2'-exo-C-3'-endo, 2T3. The anti conformation is favored for both puckers and the conformation about the C-4'-C-5' bond shows a very slight preference for gauche-gauche in C-3'-endo-C-2'-exo and gauche-trans in C-2'-exo-C-3'-endo. In the corresponding 5'-nucleotide, the anti-gg combination is strongly favored for the C-3'-endo pucker while it constitutes <50% for the C-2'-exo pucker. The C-2'-exo rings favor lower values (<0.degree.) of glycosyl torsions than the C-3'-endo rings. While 2'-O-methylation has little effect on the preferred conformations of either the nucleosides or 5'-nucleotides, the range of favored conformations of the 3'-phosphate group is considerably restricted. The conformation of the Me group itself is restricted to values of 80-160.degree. in nucleosides and 5'-nucleotides and is further constrained to values 90-130.degree. in the presence of the 3'-phosphate.

IT **54619-24-8**
RL: PRP (Properties)
(conformation of, effect of ribose methylation on)
RN 54619-24-8 CAPLUS
CN 3'-Adenylic acid, 2'-O-methyl-, 5'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



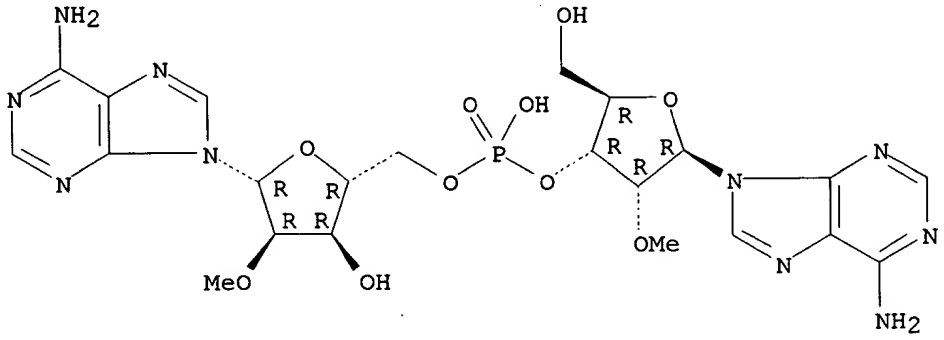
L51 ANSWER 27 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1975:31477 CAPLUS
DOCUMENT NUMBER: 82:31477
TITLE: Optical studies of the base-stacking properties of 2'-O-methylated dinucleoside monophosphates
AUTHOR(S): Drake, A. F.; Mason, S. F.; Trim, A. R.
CORPORATE SOURCE: Chem. Dep., King's Coll., London, Engl.
SOURCE: J. Mol. Biol. (1974), 86(4), 727-39
CODEN: JMOBAK
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of 2'-O-methylation on the base-stacking properties of 13 dinucleoside monophosphates was studied by CD measurements at -20 to +80.degree. at high and low salt concns. in neutral aq. soln. E.g., methylation, which generally enhanced the stacking propensity of dinucleoside monophosphates, inhibited stacking in dimers with adenine in the 3'-linked nucleoside. The effects of salt concns., suggested that the 2'-OMe effected stacking by displacing ions from the immediate environment of the dimer as well as by intermol. steric effects. The role of modified nucleosides in the conformation of RNAs is discussed in relation to these data.

IT **54621-66-8 54621-67-9 54621-68-0**
RL: PRP (Properties)
(CD spectrum of, base-stacking in relation to)

RN 54621-66-8 CAPLUS
CN Adenosine, 2'-O-methyladenylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

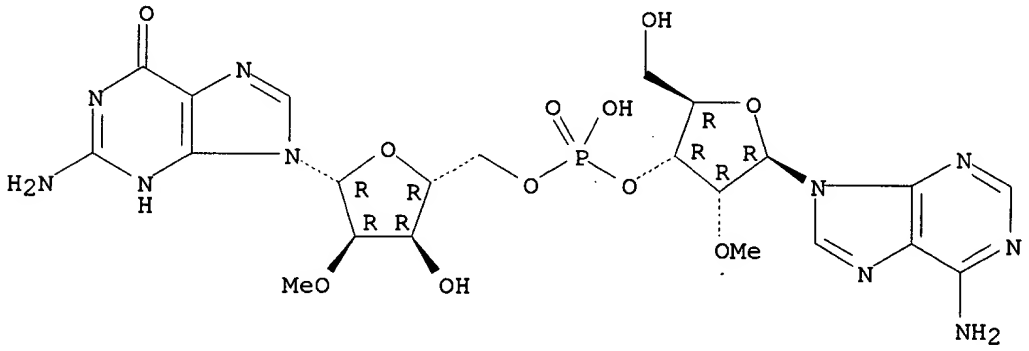
Absolute stereochemistry.



RN 54621-67-9 CAPLUS
CN Guanosine, 2'-O-methyladenylyl-(3'.fwdarw.5')-2'-O-methyl- (9CI) (CA INDEX NAME)

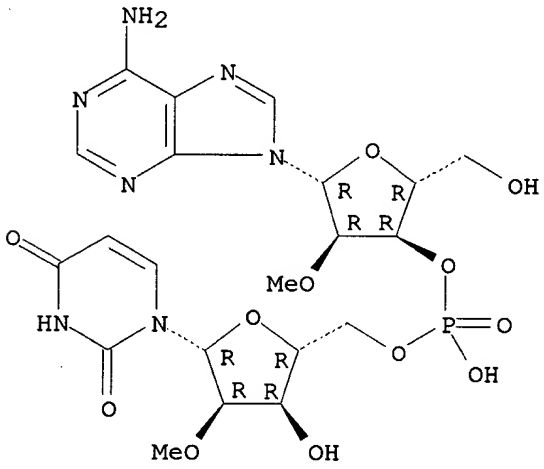
Searched by Barb O'Bryen, STIC 308-4291

Absolute stereochemistry.



RN 54621-68-0 CAPLUS
CN Adenosine, 2'-O-methyluridylyl-(5'.fwdarw.3')-2'-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

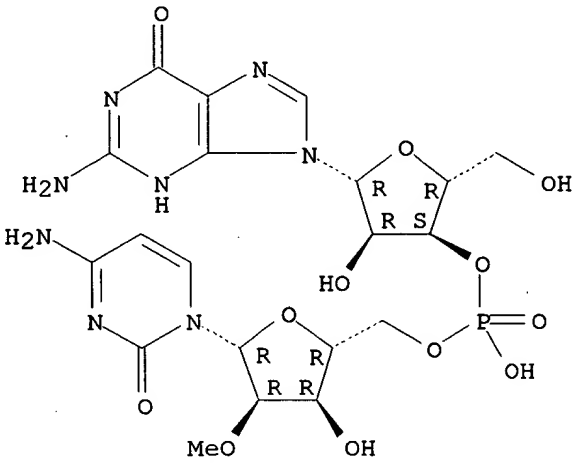


L51 ANSWER 28 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1974:146455 CAPLUS
DOCUMENT NUMBER: 80:146455
TITLE: Oligoribonucleotide synthesis. VII. Synthesis of the anticodon loop of Escherichia coli methionine transfer ribonucleic acid
AUTHOR(S): Neilson, T.; Werstiuk, E. S.
CORPORATE SOURCE: Dep. Biochem., McMaster Univ., Hamilton, Ont., Can.
SOURCE: J. Amer. Chem. Soc. (1974), 96(7), 2295-7
CODEN: JACSAT
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nonaribonucleotide, GCmUCAUAAC (m = methionine), was synthesized using a block phosphotriester method. Its sequence is identical to that of the anticodon loop of transfer RNAfMet (E. coli). Protected di- and trinucleotides, GCm, UC, AUA, AC, assembled stepwise from nucleoside derivs., were joined together to give protected tetramer, GCmUC, and pentamer, AUAAC. Linkage of these fragments followed by deblocking, gave the free nonomer in mg. amts.
IT **52571-48-9P**

Searched by Barb O'Bryen, STIC 308-4291

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 52571-48-9 CAPLUS
CN Guanosine, 2'-O-methylcytidylyl-(5'.fwdarw.3')- (9CI) (CA INDEX NAME)

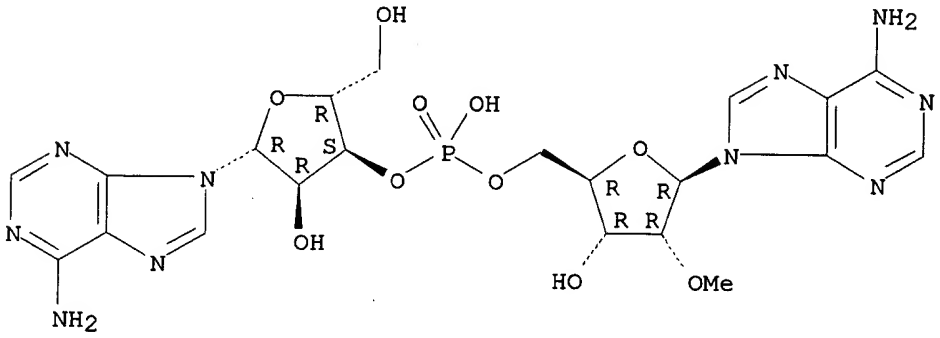
Absolute stereochemistry.



L51 ANSWER 29 OF 29 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1969:418774 CAPLUS
DOCUMENT NUMBER: 71:18774
TITLE: Optical activity of single-stranded polydeoxyadenylic and polyriboadenylic acids; dependence of adenine chromophore Cotton effects on polymer conformation
AUTHOR(S): Bush, C. Allen; Scheraga, Harold A.
CORPORATE SOURCE: Cornell Univ., Ithaca, N. Y., USA
SOURCE: Biopolymers (1969), 7(3), 395-409
CODEN: BIPMAA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Circular dichroism (CD) curves are reported for poly dA, (pdA)6, (pdA)2 poly A, ApAp, ApA, AMP, dApA, pdApA, A-2'-O-methyl-pA, and A-2'-O-methyl-pAp. Single CD bands at 228-230 m.mu. and at 278-280 m.mu. occurred in oligomers longer than dinucleotides. In the case of dinucleotides and mononucleotides, the 230 m.mu. CD of band appears but the 280 M.mu. CD band does not. The 230 m.mu. band is assigned to a very weak .pi.-.pi.* transition at this wavelength. Theoretical considerations show that the 280 m.mu. band is not an exciton component of the strong .pi.-.pi.* transition at 260 m.mu. in adenine. It was concluded that the 280 m.mu. CD band must be assigned to a distinct absorption, probably arising from an n-.pi.* transition. The fact that the n-.pi.* CD band at 280 m.mu. is not seen in mononucleotides or dinucleotides is ascribed to solvation of the adenine ring by water, which shifts the band to shorter wavelengths. Therefore, only interior residues of oligomers have the 280 m.mu. band, and the optical activity of a polymer cannot be computed from that of a dinucleotide by using a nearest-neighbor approxn. The existence of this end effect has been tested, by taking it into account in computing the rotational strengths of the 278 m.mu. n-.pi.* transition for several oligomers; a more sensitive test of this end effect would require CD data for the oligo dA series of 3 to 5 residues. The structural and optical differences between poly dA and poly A, and the need for a theoretical treatment of n-.pi.* Cotton effects in polynucleotides, are discussed.
IT **26350-95-8**
RL: PRP (Properties)

(dichroism of, circular)
RN 26350-95-8 CAPLUS
CN Adenosine, 5'-adenylyl-(3'.fwdarw.5')-2'-O-methyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



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